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

Rainer Birringer
Universität des Saarlandes
Technische Physik, Gebäude D2 2
D-66041 Saarbrücken
r.birringer@nano.uni-saarland.de

German Society of Materials Science and Engineering
Bundesvereinigung Materialwissenschaft und Werkstofftechnik

Dieter M. Herlach
Deutsches Zentrum für Luft- und Raumfahrt e.V.
Institut für Materialphysik im Weltraum
D-51147 Köln
dieter.herlach@dlr.de

Overview of Invited Talks and Sessions

(lecture rooms H4, H5, H6 and H16; Poster C)

Invited Talks

MM 9.1	Mon	14:00–14:30	H16	**Dynamic arrest in multicomponent glass forming alloys** — •Franz Faupel, Alexander Bartsch, Klaus Rätzke, Andreas Meyer
MM 17.1	Tue	9:30–10:00	H16	**Interfaces in nanostructured matter** — •Guido Schmitz
MM 25.1	Tue	14:00–14:30	H16	**Models for ductile fracture and their application to forming processes** — •Hermann Riedel
MM 27.1	Wed	9:30–10:00	H16	**Multiferroic Composites** — •Dwight Viehland
MM 36.1	Wed	14:00–14:30	H16	**Atomistic simulations of plastic deformation - insights from a quantitative approach** — •Erik Bitzek
MM 45.1	Thu	9:30–10:00	H16	**"Novel" Materials for Lithium Ion Batteries and "Beyond-Lithium Ion Batteries"** — •Martin Winter, Stefano Passerini

Invited talks of the joint symposium SYGN

See SYGN for the full program of the Symposium.

SYGN 1.1	Mon	14:00–14:35	H1	**Models for spin-orbit coupling in graphene** — •Francisco Guinea
SYGN 1.2	Mon	14:35–15:10	H1	**Spin-orbit coupling and spin relaxation in carbon nanotube quantum dots** — •Ferdinand Kuemmeth
SYGN 1.3	Mon	15:10–15:45	H1	**Spin-orbit interaction in carbon nanotubes probed in pulsed magnetic fields** — •Sungho Jhang, Magdalena Marganska, Yurii Skourski, Dominik Preusche, Benoit Witkamp, Milena Grifoni, Herre van der Zant, Joachim Wosnitza, Christoph Strunk
SYGN 1.4	Mon	16:00–16:35	H1	**Wigner molecules and spin-orbit coupling in carbon-nanotube quantum dots** — •Massimo Rontani
SYGN 1.5	Mon	16:35–17:10	H1	**Spin relaxation and decoherence in graphene quantum dots** — •Guido Burkard
SYGN 1.6	Mon	17:10–17:45	H1	**Spin transport in graphene field effect transistors** — •Bart van Wees

Invited talks of the joint symposium SYAT

See SYAT for the full program of the Symposium.

SYAT 1.1	Wed	14:30–15:00	H1	**Aging, ergodicity breaking and universal fluctuations in continuous time random walks: Theory and (possible) experimental manifestations** — •Igor Sokolov
SYAT 1.2	Wed	15:00–15:30	H1	**Distinguishing anomalous from simple diffusion in crowded solutions and in cells with fluorescence correlation spectroscopy** — •Cecile Fradin, Daniel Banks, Shyemaa Shehata, Felix Wong, Robert Peters
SYAT 1.3	Wed	15:30–16:00	H1	**Exploring Diffusion in Nanostructured Systems with Single Molecule Probes: From Nanoporous Materials to Living Cells** — •Christoph Bräuchle
SYAT 2.1	Wed	16:30–17:00	H1	**The Lorentz model: a paradigm of anomalous transport** — •Felix Höfling
SYAT 2.2	Wed	17:00–17:30	H1	**Viscoelastic subdiffusion: from anomalous to normal** — •Igor Goychuk
SYAT 2.3	Wed	17:30–18:00	H1	**Phase transitions, liquid micro-compartments, and embryonic patterning** — •Clifford Brangwynne, Jöbin Gharakhani, Anthony Hyman, Frank Jülicher

Invited talks of the joint symposium SYNT

See SYNT for the full program of the Symposium.

SYNT 1.1	Fri	10:15–10:45	H1	**Atomic friction under ultrahigh vacuum conditions** — •Ernst Meyer, Enrico Gnecco, Pascal Steiner, Gregor Fessler, Sascha Koch, Thilo Glatzel, Alexis Baratoff, Mircin Kisiel, Urs Gysin, Akshata Rao, Shigeki Kawai, Sabine Maier
SYNT 1.2	Fri	10:45–11:15	H1	**Layering and Squeeze-out Damping in Confined Liquid Films** — •Frieder Mugele
SYNT 1.3	Fri	11:15–11:45	H1	**Wear on the nanoscale: mechanisms and materials** — •Bernd Gotsmann, Mark A. Lantz, Harish Bhskaran, Abu Sebastian, Ute Drechsler, Michel Despont, Yun Chen, Kumar Sridharan, Papot Jaroenapibal, Robert Carpick
SYNT 1.4	Fri	11:45–12:15	H1	**Friction at the Nanoscale: Insights from Atomistic Simulations** — •Izabela Szlufarska, Yifei Mo, Yun Liu, Maneesh Mishra
SYNT 1.5	Fri	12:15–12:45	H1	**The friction of wrinkles** — •Martin H. Müser, Hamid Mohammadi
SYNT 1.6	Fri	12:45–13:15	H1	**Influence of humidity on nano- and micromechanical contact adhesion** — •Hans-Jürgen Butt

Topical Sessions (MM)

Glass Dynamics (GD)

Glasses and liquids are inhomogeneous on atomic length scales and are characterized by disordered atomic configurations which vary in space on the nanometer scale. Dynamic properties such as structural relaxation and diffusion are important topics in glass research, applying to oxide, polymeric and metallic glasses. The mechanical properties of glasses result generally from inhomogeneous deformation via shear bands and often involve different length scales, ranging from the atomic to the micrometer scale. Thus, the structure, dynamics and the resulting properties of glasses involve in many cases great ranges in length and time scales, and bridging them is an important problem in glass research which is seeking solutions.

This symposium aims to bring together scientists from different research communities, i.e. the fields of metallic, oxide, and polymeric glasses, and colloidal systems. The similarities among and differences between these glassy systems will be an emphasis, with the aim of finding common, fundamental mechanisms in glasses and understanding in more detail the nature of the glass transition.

Organizers:
Prof. Dr. Jörg Löffler
Eidgenössische Technische Hochschule Zürich, Metal Physics and Technology, Wolfgang-Pauli-Str. 10, CH 8093 Zürich
Prof. Dr. Andreas Meyer
Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Linder Höhe, D-51147 Köln

Multifunctional Materials (MfM)

Modern, technological, smart applications require new functionalities of surfaces or interfaces - multifunctional materials serve more than simply a structural purpose, they perform at least one additional function. Examples include but are not limited to: transparent or flexible conductors, multiferroic materials, damage tolerant materials, sensing and actuating systems, self healing systems, and nanocomposites or nanostructured materials with antibacterial, anti-reflecting or anti-fogging properties. To design these multifunctional materials, a detailed understanding of the basic physics and materials science of underlying surface, interface, and micro- or nanostructures is necessary.

The symposium is intended as a forum for researchers to present their contributions to multifunctional materials ranging from the basic research, for example of functional layers or nanostructures, to the effects in applications. Oral and poster contributions to the symposium related to experiment or theory are highly welcome. The field of multifunctional materials is interdisciplinary and encompasses all stages of research from fundamental understanding to application and is of an interdisciplinary nature, offering promising opportunities for research collaborations.

Organizer:
Prof. Dr. Rainer Adelung
Christian-Albrechts-University Kiel, Institute for Materials Science, Kaiserstr. 2, D-24143 Kiel

Physical Properties and Mechanisms in Battery Materials (BM)

Designing materials with specific combinations of properties is a challenging step in the development of high energy and high power density batteries. The efficiency as well as reproducibility and reliability of energy conversion and storage are determined by the properties of the battery components, in particular of the electrodes, the separator and the respective interfaces.

This symposium will focus on critical materials issues in developing better battery electrodes and membranes.

Organizers:
Prof. Dr. Guido Schmitz
Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster
Prof. Dr. Cynthia A. Volkert
Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Joined Topical Session (MM, KR and BV MatWerk)

Photovoltaic Materials (PM)

In Central Europe, photovoltaic energy conversion from solar cells has by far the greatest proven technological potential for the production of electricity from renewable energy sources. Therefore the symposium is devoted to materials science problems in photovoltaics, especialley related to structure-property relations of photovoltaic materials.

Organizer:
Prof. Dr. Susan Schorr
Freie Universität Berlin, FB Geowissenschaften, Malteserstr. 74-100, 12249 Berlin

Topical Sessions (BV MatWerk)

Growth Kinetics of Bulk Crystals, Thin Films, and Nanostructures (GK)

Kinetic processes play an important role in the growth of single crystals, the solidification of multi-crystalline material, and the deposition of thin films and nanostructures. Often they have a direct impact on the properties of the final product and thus an understanding of these processes is required for improving existing materials as well as for developing new ones. The goal of this symposium is to bring together scientists from different disciplines in order to present and to discuss current topics of growth kinetics.

Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, DGKK
Organizers:
Dr. Wolfram Miller
Leibniz Institut für Kristallwachstum, Max-Born-Straße 2, D-12489 Berlin
Prof. Dr. Joachim Krug
Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str. 77, D-50937 Köln

Prof. Dr. Thomas Michely
Universität zu Köln, II. Physikalisches Institut, Zülpicher Str. 77, D-50937 Köln

Designing innovative structural materials and steels based on computational and experimental simulations (DISM)
The realization and success of Green Technologies is closely related to the availability of innovative structural materials as, e.g., high-strength and/or high-temperature resistant steels. Such materials are for instance highly desired in car manufacturing, where they simultaneously allow weight-reduction and an improvement of passenger safety, as well as in power stations, where an increase in operating temperatures in turbines yields a boost in efficiency. In contrast to common steels, advanced structural materials exhibit a surprisingly complex phase composition, chemistry and microstructure. With increasing complexity, however, traditional empirically driven materials design becomes less and less effective. In order to address this challenge, presently a new generation of simulation approaches is under development. These approaches are inherently hierarchical and interdisciplinary by nature and combine engineering with physics, chemistry and applied mathematics. The objective of this symposium is to provide an overview about recent developments and emerging new activities in this field, to provide a platform that brings together experts of the various related fields, and to allow young scientists to learn more about this fascinating and rapidly growing research area.
Technical association for Iron Metallurgy - Stahlinstitut VDEh
Organizer:
Prof. Dr. Jörg Neugebauer
Max-Planck-Institut für Eisenforschung, Computational Materials Design, Max-Planck-Strasse 1, D-40237 Düsseldorf

Nachwuchskarriereworkshop (BV MatWerk und MM)

Doktorprüfung bestanden, Doktorfeier überstanden, Formalitäten abgeschlossen. Nun stehen Sie als frischgebackener Doktor da und was nun? Vielleicht sollen Sie morgen eine Stelle in einem Forschungsinstitut oder in der Industrie antreten. Was erwartet Sie dort? Welche Fähigketen und Erfahrungen werden Ihnen bei der Einarbeitung hilfreich sein? Was erwarten Ihre Vorgesetzten, Ihre Kollegen von Ihnen? Welche Karriere sollen Sie einschlagen, Hochschule oder Industrie? Der Wechsel vom überschaubaren Alltag als Doktorand an der Universität zum Berufsleben stellt eine Zäsur im Leben jedes Wissenschaftlers dar und verlangt eine überlegte Entscheidung.
Die Bundesvereinigung Materialwissenschaft und Werkstofftechnik (BV MatWerk) und der Fachverband Metall- und Materialphysik wollen Ihnen mit einem Karriereworkshop bei diesen Entscheidungsprozessen helfen: Darin werden Kolleginnen und Kollegen aus Ihren Erfahrungen in der privaten Wirtschaft, in außeruniversitären Forschungseinrichtungen und in der Professorenlaufbahn berichten und Ihre Fragen beantworten.

Dienstag, 23. März 2010, 14:00 - 18:00 Uhr, Hörsaal H4

Sessions

MM 1.1–1.3	Mon	10:15–11:30	H16	**Topical Session Glass Dynamics I**
MM 2.1–2.3	Mon	12:00–13:00	H16	**Topical Session Glass Dynamics II**
MM 3.1–3.2	Mon	10:15–11:15	H4	**Topical Session Designing Innovative Structural Materials and Steels I**
MM 4.1–4.5	Mon	11:30–12:45	H4	**Topical Session Designing Innovative Structural Materials and Steels II**
MM 5.1–5.4	Mon	10:15–11:15	H6	**Diffusion and Point Defects I**
MM 6.1–6.4	Mon	11:30–12:30	H6	**Diffusion and Point Defects II**
MM 7.1–7.4	Mon	10:15–11:15	H5	**Intermetallic Phases I**
MM 8.1–8.4	Mon	11:30–12:30	H5	**Intermetallic Phases II**
MM 9.1–9.1	Mon	14:00–14:30	H16	**HV Faupel**
MM 10.1–10.2	Mon	14:45–15:30	H16	**Topical Session Glass Dynamics III**
MM 11.1–11.4	Mon	16:00–17:30	H16	**Topical Session Glass Dynamics IV**
MM 12.1–12.4	Mon	14:45–15:45	H4	**Topical Session Designing Innovative Structural Materials and Steels III**

MM 13.1–13.7	Mon	16:00–17:45	H4	**Topical Session Designing Innovative Structural Materials and Steels IV**
MM 14.1–14.4	Mon	14:45–15:45	H6	**Diffusion and Point Defects III**
MM 15.1–15.5	Mon	14:45–16:00	H5	**Interfaces I**
MM 16.1–16.3	Mon	16:15–17:00	H5	**Interfaces II**
MM 17.1–17.1	Tue	9:30–10:00	H16	**HV Schmitz**
MM 18.1–18.3	Tue	10:15–11:15	H16	**Topical Session Glass Dynamics V**
MM 19.1–19.2	Tue	10:15–11:15	H4	**Topical Session Designing Innovative Structural Materials and Steels V**
MM 20.1–20.6	Tue	11:30–13:00	H4	**Topical Session Designing Innovative Structural Materials and Steels VI**
MM 21.1–21.5	Tue	10:15–11:30	H6	**Mechanical Properties I**
MM 22.1–22.5	Tue	10:15–11:30	H5	**Hydrogen in Metals**
MM 23.1–23.3	Tue	11:45–12:30	H5	**Quasicrystals**
MM 24.1–24.1	Tue	13:30–13:45	H16	**BV Matwerk**
MM 25.1–25.1	Tue	14:00–14:30	H16	**HV Riedel**
MM 26.1–26.82	Tue	14:45–16:30	Poster C	**Poster Session**
MM 27.1–27.1	Wed	9:30–10:00	H16	**HV Viehland**
MM 28.1–28.6	Wed	10:15–11:45	H16	**Nanostructured Materials I**
MM 29.1–29.4	Wed	12:00–13:00	H16	**Nanostructured Materials II**
MM 30.1–30.4	Wed	10:15–11:30	H4	**Topical Session Photovoltaic Materials I**
MM 31.1–31.6	Wed	11:45–13:15	H4	**Topical Session Photovoltaic Materials II**
MM 32.1–32.4	Wed	10:15–11:45	H6	**Topical Session Multifunctional Materials I**
MM 33.1–33.3	Wed	12:00–13:00	H6	**Topical Session Multifunctional Materials II**
MM 34.1–34.4	Wed	10:15–11:15	H5	**Liquid and Amorphous Metals I**
MM 35.1–35.4	Wed	11:30–12:30	H5	**Liquid and Amorphous Metals II**
MM 36.1–36.1	Wed	14:00–14:30	H16	**HV Bitzek**
MM 37.1–37.6	Wed	14:45–16:15	H16	**Mechanical Properties II**
MM 38.1–38.6	Wed	16:30–18:00	H16	**Mechanical Properties III**
MM 39.1–39.4	Wed	14:45–15:45	H4	**Topical Session Photovoltaic Materials III**
MM 40.1–40.3	Wed	16:00–17:00	H4	**Topical Session Growth Kinetics I**
MM 41.1–41.4	Wed	17:15–18:15	H4	**Topical Session Growth Kinetics II**
MM 42.1–42.4	Wed	14:45–16:15	H6	**Topical Session Multifunctional Materials III**
MM 43.1–43.5	Wed	14:45–16:00	H5	**Materials Design I**
MM 44.1–44.4	Wed	16:15–17:15	H5	**Materials Design II**
MM 45.1–45.1	Thu	9:30–10:00	H16	**HV Winter**
MM 46.1–46.6	Thu	10:15–11:45	H16	**Nanostructured Materials III**
MM 47.1–47.4	Thu	10:15–11:30	H4	**Topical Session Growth Kinetics III**
MM 48.1–48.4	Thu	11:45–13:00	H4	**Topical Session Growth Kinetics IV**
MM 49.1–49.4	Thu	10:15–11:45	H6	**Topical Session Battery Materials I**
MM 50.1–50.2	Thu	12:15–13:00	H6	**Topical Session Battery Materials II**
MM 51.1–51.4	Thu	10:15–11:15	H5	**Electronic Properties I**
MM 52.1–52.6	Thu	11:30–13:00	H5	**Electronic Properties II**
MM 53.1–53.4	Thu	14:00–15:00	H16	**Nanostructured Materials IV**
MM 54.1–54.7	Thu	15:15–17:00	H16	**Nanostructured Materials V**
MM 55.1–55.5	Thu	14:00–15:15	H4	**Topical Session Growth Kinetics V**
MM 56.1–56.6	Thu	15:30–17:00	H4	**Topical Session Growth Kinetics VI**
MM 57.1–57.5	Thu	14:00–15:30	H6	**Topical Session Battery Materials III**
MM 58.1–58.5	Thu	15:45–17:30	H6	**Topical Session Battery Materials IV**
MM 59.1–59.5	Thu	14:00–15:15	H5	**Phase Transitions I**
MM 60.1–60.6	Thu	15:30–17:00	H5	**Phase Transitions II**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 18:30–19:30 H6

- Report of the chairman of the Metal and Material Physics Division.
- Election of the new chairman of the Metal and Material Physics Division.
- Invited talks and symposia for the next spring meeting 2011.
- Other topics.

MM 1: Topical Session Glass Dynamics I

Time: Monday 10:15–11:30 Location: H16

Topical Talk MM 1.1 Mon 10:15 H16

Colloidal Liquids and Glasses under Shear — •Stefan Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine-University, 40225 Düsseldorf, Germany

Colloidal liquids and glasses have been investigated experimentally. They consist of hard-sphere colloids with a short-range attraction induced by the depletion effect of non-adsorbing polymers, which allows us to control the range and strength of the particle-particle interactions. In these systems, liquid and crystalline states represent the equilibrium phases, while non-equilibrium, arrested states are observed at high colloid and/or polymer concentrations.

We have investigated the behaviour of these non-equilibrium states under shear. They were subjected to oscillatory shear as well as switch-on and switch-off of steady shear flow. The effect of shear on the structure and dynamics of the particles was determined. Due to their size, the particle motion can be followed using confocal microscopy and their dynamics quantified by, e.g., the mean-squared displacements. The transient dynamics show super-diffusive motion at intermediate times. These results are compared to recent simulations and theoretical predictions.

Topical Talk MM 1.2 Mon 10:45 H16

Relaxation and flow in glassy colloids — •Hans M. Wyss[1,2], Johan Mattsson[1,3], Alberto Fernandez-Nieves[1,4], Kunimasa Miyazaki[5,6], Zhibing Hu[7], David R. Reichman[5], and David A. Weitz[1] — [1]Harvard University, Cambridge, USA — [2]TU Eindhoven, Eindhoven, Netherlands — [3]Chalmers University, Gothenburg, Sweden — [4]Georgia Tech, Atlanta, USA — [5]Columbia University, New York, USA — [6]Tsukuba University, Tsukuba, Japan — [7]University of North Texas, Denton, USA

For different molecular glass-forming liquids, the dynamics of glass formation show broad variations, as often characterized by the concept of fragility - the sensitivity of the viscosity or structural relaxation time on temperature as the glass is approached. Glass formation can also be studied in colloidal materials, where increasing concentration has an effect analogous to decreasing the temperature in molecular liquids. However, in this analogy only highly fragile behavior has been observed.

In this talk I will show that by using soft, deformable particles the concept of fragility can be extended to colloidal glasses. We capture the entire range of dynamic behaviors merely by varying the softness of the individual mesoscopic particles. Hard particles make "fragile" glasses and soft particles make non-fragile, or "strong", glasses. Remarkably, we find that elasticity has an equivalent effect in molecular systems, where elasticity directly reflects fragility. I will further show how in colloids an externally enforced flow can be used to further study the structural relaxation in these materials.

MM 1.3 Mon 11:15 H16

Dynamics of colloidal suspensions in a modulated light field — •Cecile Dalle-Ferrier, Matthew Jenkins, and Stefan Egelhaaf — Lehrstuhl für Physik der weichen Materie, Heinrich Heine Universität, Düsseldorf, Deutschland

We experimentally investigated the structure and dynamics of an aqueous suspension of charged polystyrene beads in a modulated light field. The light field can be considered as an external 1D-periodically modulated potential, which has been shown to be a good model for the non-Gaussian dynamics in glassy systems of cage escape and subsequent recaging [1]. Our samples indeed showed glassy behaviour in the modulated light field, even in the case of dilute samples. Following the particles with microscopy, we find that the time-dependence of the mean-square displacement exhibits a plateau and the value of the non-gaussian parameter is non-zero. The height of the plateau and its extension in time, and more generally the dynamics of the particles, depend on the characteristics of the potential such as its amplitude and period. These results indicate that the application of a modulated light field to a colloidal suspension is a convenient tool to turn a liquid into a glass-like system. It offers extensive control of this transition through the parameters of the light field. We plan to use this model further to progress our understanding of the glass transition, in particular the characterization of glassy dynamics, including dynamical heterogeneities.

[1] B. Vorselaars et al., Non-Gaussian nature of glassy dynamics by cage to cage motion, Phys. Rev. E, 75, 011504 (2007)

MM 2: Topical Session Glass Dynamics II

Time: Monday 12:00–13:00 Location: H16

Topical Talk MM 2.1 Mon 12:00 H16

Nanomechanics of glasses and supercooled melts — •S. G. Mayr — Leibniz-Institut für Oberflächenmodifizierung e.V. — Translationszentrum für regenerative Medizin, Universität Leipzig — Fakultät für Physik und Geowissenschaften, Universität Leipzig

Metallic glasses are characterized by a rather complex viscoelastic response and the occurrence of the glass transition, while the underlying atomistic foundations are still poorly understood. Using a realistic CuTi model glass we employ global and local elasticity tensors for a thorough analysis of relaxation kinetics and mechanical stability at the nanoscale. We obtain strong indication [1] that i) α and β relaxation are closely related, presumably manifestations of a general relaxation scenario, ii) glasses reveal intrinsic mechanical instabilities at the nanoscale, which are closely connected to collective shear events within shear transformation zones and iii) the glass transition can be understood as a percolation transition of these mechanically unstable regions.

[1] S.G. Mayr, Phys. Rev. B 79, 060201(R) (2009)

This research is funded by the German DFG-PAK 36.

MM 2.2 Mon 12:30 H16

Temperature dependent shear band dynamics in a Zr-based bulk metallic glass — •David Klaumünzer, Robert Maass, Florian Dalla Torre, and Jörg Löffler — Laboratory of Metal Physics and Technology, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland

There is strong interest in determining the time scales involved in the shear banding process during plastic deformation of bulk metallic glasses. Knowing these time scales helps to understand shear banding in more detail, and may also answer the question of whether significant localised heating can occur in and near shear bands. In this study we investigated flow serrations, corresponding to discrete shear events, of a $Zr_{52.2}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$ (Vit105) bulk metallic glass with respect to their stress drop and strain burst magnitude as well as their duration, as a function of temperature in the range of 60°C to -40°C. The results show that while the stress drop magnitude and the strain burst magnitude remain approximately constant with varying temperature, there is a strong temperature dependence of the shear event duration, ranging from approximately 1 ms at 60°C to 80 ms at -40°C. A calculation of the associated shear band velocities shows pronounced Arrhenius-type behaviour with an activation energy of 0.3 eV, in good agreement with recent potential energy landscape simulations. The strong temperature dependence of shear banding observed in this metallic glass is found to be analogous to the behaviour of other (non-metallic) amorphous materials.

MM 2.3 Mon 12:45 H16

Deformation mechanisms in small samples of $Pd_{77}Si_{23}$ metallic glass — •Dominik Tönnies[1], Frans Spaepen[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

Bulk metallic glasses show some remarkable mechanical properties, but their poor plastic behavior at room temperature limits their use in applications. In recent studies, the size dependence of room temperature deformation mechanisms has been investigated by micro-compression tests on a $Pd_{77}Si_{23}$ metallic glass. The results show a clear transition from the expected mechanism of shear band formation to homogeneous deformation in pillars with diameters smaller than 440 nm. In an effort to understand the parameters that control this size transition, further micro-compression and nanoindentation studies have been performed on the $Pd_{77}Si_{23}$ films as a function of the extent of structural relaxation. The results show that in a relaxed sample the critical transition size for homogeneous deformation is reduced. The results will be discussed in terms of sample size-dependent shear band spacing and overlap.

MM 3: Topical Session Designing Innovative Structural Materials and Steels I

Time: Monday 10:15–11:15 Location: H4

Topical Talk MM 3.1 Mon 10:15 H4

Materials design for new cold formable steels — •Wolfgang Bleck — Department of Ferrous Metallurgy, RWTH Aachen University, Intzestr. 1, 52072 Aachen

Optimising the balance of strength and formability is one of the major topics in current sheet steel development. In addition to the empirical approaches new design methods based on computational engineering have been developed and are currently being applied. Different modelling options are being discussed with respect to their prediction capability, their quantitative accuracy and their limitations. Examples are provided focusing on the recent development of car body steels.

Topical Talk MM 3.2 Mon 10:45 H4

The long way from "atom to auto": Materials Simulation today — •Ingo Steinbach — Stiepelerstrasse 129 44801 Bochum

The possibility to build a material from its constituents, the atomic cores and electrons, on a computer at finite temperatures inspires the imagination of materials scientists from academic research as well as from industry. In a hierarchical approach information from the electronic and atomistic scale can be transformed to defect structures on a mesoscopic scale, the knowledge of which is crucial for advanced materials descriptions on the macroscopic scale. An alternative approach, and even more ambitious, is the concurrent multiscale method which aims on representing multiple scales in one calculation. A well known application is propagation of a crack tip where the mechanical load on a work piece is transferred by seamless combinations of materials models down to the atomic bonds. The reason to formulate these hierarchies and combinations of models is obviously the impossibility to represent the whole work piece by atoms in today's (and tomorrow's) computers. The talk will review the state of the art of modern multiscale materials simulation and highlights new developments from the author's own research.

MM 4: Topical Session Designing Innovative Structural Materials and Steels II

Time: Monday 11:30–12:45 Location: H4

MM 4.1 Mon 11:30 H4

From atoms to materials: one billion atoms with DFT accuracy — •Tobias Kerscher[1], Stefan Müller[1], Gus Hart[2], and Quinn Snell[3] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany — [2]Brigham Young University, Department of Physics and Astronomy, Provo UT 84602, USA — [3]Brigham Young University, Computer Science Department, Provo UT 84602, USA

We use an ab-initio-based cluster-expansion Hamiltonian (see e.g. [1]) to bridge the gap in length-scales between atomistic density-functional calculations ($\sim 10^3$ atoms at $T = 0$ K) and macroscopic materials ($\sim 10^9$ atoms at $T > 0$ K). To this end, our code UNCLE [2] comprises a weak-scaling parallel Monte-Carlo algorithm, which enables us to perform large-scale simulations with the cluster-expansion's ab-initio precision. We demonstrate the effectiveness of the algorithm by a simple 2d Ising model, and apply it on the macroscopic scale ($\sim 0.3\,\mu$m) to the ternary bulk system $Ni_{48}Al_{50}$ with one billion atomic sites.
Supported by Deutsche Forschungsgemeinschaft

[1] S. Müller, J. Phys.: Condens. Matter **15** (2003), R1429
[2] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

MM 4.2 Mon 11:45 H4

From DFT via TB to BOP: Atomistic simulations with abinitio derived bond order potentials — •Martin Reese[1,2], Matous Mrovec[1,2], Bernd Meyer[3], and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [2]IZBS, Universität Karlsruhe — [3]ICMM, Universität Erlangen-Nürnberg

Nanostructered composites of crystalline and amorphous carbides and nitrides can yield materials that reach the limit of super-hardness. These unusual properties are related to a subtle balance between the amorphous and crystalline phases and the properties of interfaces at the nanometer level. Atomistic simulations can significantly contribute to a better understanding of these complex materials provided that the employed models of atomic interactions are robust and reliable.

In this work we present a bottom-up procedure, which enables a development of ab-initio derived analytic bond-order potentials (BOPs). First, by projecting the self-consistent electronic wave functions from density functional theory onto a minimum basis of atomic orbitals we construct tight-binding models, which retain the crucial aspects of electronic structure. These are then further coarse-grained into a form of the interatomic BOPs, which describe correctly the interatomic bonding and are computationally efficient.

The procedure will be demonstrated for C-H and C-Si systems. The performance and transferability of the constructed BOPs on various complex structures will be presented.

MM 4.3 Mon 12:00 H4

Ab initio determination of the magnetic free energy contribution of metallic systems — •Fritz Körmann, Alexey Dick, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

An accurate prediction of the free energy is the basis to compute phase diagrams, finite temperature materials parameters, or kinetic barriers and is thus fundamental in computational materials design. One of the most challenging contributions - but crucial for many engineering materials - is the magnetic entropy. The most popular ab initio approach for the latter is the use of an effective Heisenberg model solved using classical Monte Carlo (cMC) approaches and neglecting quantum effects. We discuss the impact of the latter based on extensive model calculations where Quantum MC calculations are available. An empirical rescaling scheme is derived allowing to considerably improve the cMC. The method is applicable to strong ferromagnetic systems with magnetic frustration is absent or weak. The application and performance of the new approach is demonstrated for pure Fe.

MM 4.4 Mon 12:15 H4

Sensitivity of the stacking fault energy in FeMn alloys on the local environment: A first-principles study — •Alexey Dick, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

An in-depth understanding of the physical processes that may influence the stacking fault energy (SFE) is necessary for a knowledge-based optimization and engineering of high-Mn-steels. We have performed a first-principles study of the SFE in austenitic FeMn-alloys, which are prototype structures for realistic high-Mn-steels. The relevant atomic configurations have been identified by combination of the cluster-expansion methodology and the concept of special quasirandom structures based on the density functional theory calculations.

Employing either the axial interaction model and/or explicit calculations of the generalized SFE surfaces we show that the value of the SFE sensitively depends on type of the chemical and magnetic ordering in the system. We further show that the SFE can be changed not only by varying the composition of the FeMn-alloy or its temperature, but also by admixing different chemical elements or by controlling local strain fields.

MM 4.5 Mon 12:30 H4

DFT-based calculation of temperature-dependent stacking fault energy in the Fe-Mn alloy — •Andrei Reyes-Huamantinco[1,2], Andrei Ruban[3], Peter Puschnig[1], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Austria — [3]Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden

We have studied the Fe-22.5at.%Mn alloy in the temperature range between 300 and 800 K. The random alloy in the paramagnetic state was modelled by the coherent potential approximation (CPA) and the disordered local moment (DLM) approach. The DFT-calculations were carried out using the exact muffin-tin orbitals (EMTO) method. Temperature-dependent lattice parameter and local magnetic moment were used in constrained DFT-calculations. The former was obtained from measurements, while the latter was calculated through a longitudinal spin-fluctuation (LSF) Hamiltonian in combination with Monte Carlo simulations. The stacking fault energy (SFE) was expanded in terms of free energies of the fcc, hcp and dhcp structures, including electronic and magnetic entropies. We find that the SFE increases by 17 mJ/m^2 between 300 and 600 K, and that the hcp/fcc transformation temperature is 390 K, in agreement with experiments.

MM 5: Diffusion and Point Defects I

Time: Monday 10:15–11:15 Location: H6

MM 5.1 Mon 10:15 H6

A Novel Approach to Identify the Mechanism of Gold Diffusion in Lead — •Nico Stolwijk and Dirk Böckmann — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Fast impurity diffusion in metals has been extensively studied in the 1960s and 1970s, with Pb:Au serving as a prototype system. In particular, it was concluded from measurements of 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 Aui, Aui-vacancy pairs, or Au-Au diplons (dumbbells), however, without providing convincing evidence. Specifically, the role of substitutional Aus was not sufficiently clarified. Our experiments aim at identifying the Au diffusion mechanism by closely looking at the evolution of the Au penetration profiles in a regime of short-term isothermal annealing. To this aim, we utilise the suitability of the Pb:Au system for neutron activation analysis, which allows for the detection of diffusion profiles on an absolute concentration scale. The results are evaluated within the framework of the dissociative mechanism involving Aui-Aus exchange with the aid of vacancies.

MM 5.2 Mon 10:30 H6

The influence of Au on the decomposition of Al-Cu — •Benedikt Klobes[1], Osman Balarisi[1], Meng Liu[1], Karl Maier[1], and Torsten Staab[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn — [2]Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg

Al alloys based on the binary Al-Cu system are important structural materials since they combine light weight with high strength. Their favourable mechanical properties are induced by precipitates of nanometer size which are formed due to the vacancy driven transport of solute atoms. Usually, this precipitation process is significantly influenced by other microalloying elements, e.g. the addition of Mg accelerates and amplifies the hardness increase during ageing. In contrast, microalloying additions of Au inhibit the decomposition and age hardening of the alloy. By means of positron annihilation and x-ray absorption spectroscopy, with which the essential ingredients of age hardenable alloys, namely vacancies and solute atoms, can be probed, we show that Au atoms trap quenched-in vacancies. Since the vacancy mechanism of diffusion is surpressed this way, no age hardening can occur.

MM 5.3 Mon 10:45 H6

Zerstörungsfreie Abschätzung der Restlebensdauer an Proben des ICE-Achsstahls — •Patrick Eich[1], Reinhard Sottong[1], Matz Haaks[1], Karl Maier[1] und Hartmut Hintze[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nussallee 14-16, 53115 Bonn — [2]Deutsche Bahn AG Bahntechnikerring 74, 14774 Brandenburg-Kirchmöser

In den letzten Jahren ist das ermüdungsbedingte Versagen von Radsatzwellen im Schienenverkehr ausführlich in der Tagespresse diskutiert worden. Die heutzutage eingesetzten und an das 150 Jahre alte Wöhler-Verfahren angelehnten Methoden zur Abschätzung der Restlebensdauer erfordern sehr zeit- und kostenintensive Experimente. Aus der zerstörungsfreien Beobachtung erster Gefügeänderungen als Vorboten des Ermüdungsprozesses lässt sich vergleichbare Information mit nur ca. 1% des experimentellen Aufwandes gewinnen. Die physikalische Ursache für die Ermüdung von metallischen Werkstoffen ist die Akkumulation von Gitterfehlern, wie Versetzungen, und durch Versetzungsbewegung erzeugte Defekte. Der Aufbau der Defektdichte wird mit der Positronen-Annihilation-Spektroskopie (PAS) gemessen und so die Restlebensdauer von Stählen und Aluminiumlegierungen zerstörungsfrei bestimmt [1]. Diese Methode wurde auf Proben des ICE-Achsstahls A4T übertragen. Die Ergebnisse zeigen, dass sich aus den Frühstadien der Ermüdung die Restlebensdauer mit zu Wöhlermethoden vergleichbarer Genauigkeit abschätzen lässt.

[1] M.Haaks, K. Maier in V. Jentsch et al. "extreme events", Springer 2005

MM 5.4 Mon 11:00 H6

Fluid transport in one dimensional channel systems — •Ramona Baum, Florian Hibbe, Sergej Naumov, Jörg Kärger, and Rustem Valiullin — Department of Interface Physics, University of Leipzig, Germany

Interference microscopy (IFM) is a well-suited experimental technique for studying transport of guest molecules in nanoporous materials [1]. A sufficient spatial resolution, which is in the range of micrometers enables the monitoring of the evolution of concentration profiles under non-equilibrium conditions. The transient concentration profiles, which are the result of a change in the ambient pressure, therefore allow the study of the adsorption and desorption kinetics. L-zeolite represents an important model system to study molecular transport in nanopores. It is a crystal with a length of 7 to 8 μm with one dimensional channels arranged in a hexagonal pattern. Such organization of the pore structure allows most unambiguous verification of theoretical predictions about the diffusion process [2]. In this work, we present the data on molecular transport of propane in L-zeolite assessed using IFM. The results obtained, revealing the one dimensional character of the diffusion process, are in good correlation with the crystallographic structure of this material.

[1]L.Heinke,D.Tzoulaki, C.Chmelik, F.Hibbe, J.M.van Baten, H.Lim, J.Li, R.Krishna, J.Kärger, Phys.Rev.Lett. 102, 065901 (2009)

[2] J.Kärger, R.Valiullin, S.Vasenkov, New Journal of Physics 7 (2005) 1-15.

MM 6: Diffusion and Point Defects II

Time: Monday 11:30–12:30 Location: H6

MM 6.1 Mon 11:30 H6

Study of ^{44}Ti grain boundary self diffusion in thin nanocrystalline TiO_2 films — •Petr Straumal[1,2], Ata Myatiev[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Muenster, Germany — [2]National University of Science and Technology "MISIS", Leninsky Prospect 4, 119049 Moscow, Russia

Titanium dioxide is known for its photo-catalytic properties and enhanced corrosion resistance in aqueous environments. For catalytic applications it is helpful to dope the TiO_2 with metal dopants which can move the absorption edge of TiO_2 from the UV to the blue region of the visible spectrum. Also the electrical conductivity of non-stoichiometric TiO2 is proportional to the concentration of oxygen vacancies. The grain boundary diffusion plays a significant role in both processes. Numerous works are dedicated to the diffusion of various dopants like niobium or chromium in TiO_2 but so far, none studied the self diffusion of titanium. The grain boundary self diffusion in thin nanocrystalline TiO_2 films is investigated. The oxide films are produced using a novel deposition method from metal-organic precursors at relatively low (400-500°C) temperatures. The diffusion was measured by means of the radiotracer technique applying the ^{44}Ti isotope and utilizing ion beam sputtering for sectioning. In addition, the microstructure was investigated using TEM. The results are discussed with respect of the relationship between grain boundary self diffusion and the synthesis pathway and resulting microstructure of the nanoscale functional oxide films. Support by DAAD is gratefully acknowledged.

MM 6.2 Mon 11:45 H6

Self-diffusion of Ti and ultra fast solute diffusion of Co in annealed and severely deformed α-Ti — •Jochen Fiebig[1], Sergiy Divinski[1], Yuri Estrin[2], and Gerhard Wilde[1] — [1]Institute of Material Physics, Westfälische Wilhelms University, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Monash University, Claytoon, Victoria, Australia

Severely deformed materials attain nowadays a growing technological interest due to their advanced properties and property combination. In the present study we compared the diffusion properties, especially grain boundary diffusion, of coarse-grained and ultra fine-grained α-Ti. The severe deformation was performed by equal channel angular pressing. The radiotracer method was used in combination with the parallel sectioning technique. With this method we studied the self-diffusion of ^{44}Ti and the impurity diffusion of the so called 'fast diffuser' ^{57}Co in α-Ti before and after severe plastic deformation. For ^{57}Co ultra-fast diffusion rate along the grain boundaries in annealed α-Ti was observed which is significantly decreased after severe plastic deformation. The diffusion data is discussed with respect to the possible existence of 'non-equilibrium' grain boundaries in severely deformed materials. Support by DFG is gratefully acknowledged.

MM 6.3 Mon 12:00 H6

Untersuchung von Korngrenzen in Kupfer mithilfe eines Feinfokus-Positronen-Strahles — •Reinhard Sottong, Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Die Positronen-Annihilations-Spektroskopie (PAS) ist eine renommierte Methode zur Untersuchung von Kristalldefekten. Die Positronen dienen hierbei als Sondenteilchen, mit denen einzelne Fehlstellen beobachtbar sind.

Durch Glühen von OFC-Kupfer bei 1000°C und langsames Abkühlen auf Raumtemperatur wurden in einer Probe Körner mit einer Größe von 40 μm mal 100 μm erzeugt. Unter mechanischer Beanspruchung stellen die Korngrenzen Hindernisse für das Gleiten von Versetzungen dar, wodurch es hier zu einem Stapeln der Versetzungen kommt.

Mit der Bonner Positronen-Mikrosonde (BPM) wurde die Fehlstellendichte an einem Korn mit einer Ortsauflösung von 1 μm sowohl im unverformten Zustand als auch nach plastischer Deformation untersucht. Der Vergleich dieser Messergebnisse zeigt eine Erhöhung der Fehlstellendichte an den Korngrenzen. Positronen als Fehlstellensonden mit hoher Ortsauflösung sind ein einfaches Verfahren, um z.B. Versetzungsaufstau an Hindernissen bei schwacher Verformung zu beobachten.

MM 6.4 Mon 12:15 H6

Ultra-slow lithium diffusion in Li_3NbO_4 probed by ^{7} Li stimulated echo NMR spectroscopy — •Benjamin Ruprecht and Paul Heitjans — Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, D-30167 Hannover

Currently, a variety of fast Li conductors attract much attention due to possible future applications in batteries. In contrast, apart from fundamental aspects, for other applications such as breeder materials for fusion reactors materials with exceptionally slow Li transport are needed. We present studies on the ultra-slow Li transport in the model system Li_3NbO_4 (cubic, space group I-43m) by ^{7}Li Spin-Alignment Echo Nuclear Magnetic Resonance (SAE NMR) spectroscopy [1]. NMR spectroscopy allows one to probe ionic transport on a microscopic scale. In Li_3NbO_4 the Li ions reside in different electrical field gradients at the nuclear sites giving rise to different quadrupolar precession frequencies ω_{Q}. Diffusion induced changes of ω_{Q} during the mixing time t_{m} of the pulse sequence used lead to a decay of the stimulated echo observed. By recording the t_{m} dependence of the echo amplitude the SAE NMR experiment yields two-time single-particle correlation functions and gives direct access to correlation rates τ_{c}^{-1} which may be identified with Li jump rates [2]. In the case of Li_3NbO_4 ultra-slow lithium jumps in the regime $1..10^4\,\mathrm{s}^{-1}$ (373..553 K) were found showing that Li_3NbO_4 is indeed a very poor lithium ion conductor.

[1] R. Böhmer, K. R. Jeffrey, M. Vogel, Prog. Nucl. Magn. Reson. Spectrosc. 50 (2007) 87

[2] M. Wilkening, P. Heitjans, Solid State Ion. 177 (2006) 3031.

MM 7: Intermetallic Phases I

Time: Monday 10:15–11:15 Location: H5

MM 7.1 Mon 10:15 H5

Effective potentials for Al–Mn–Pd — •Daniel Schopf, Peter Brommer, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The Ξ-phases of Al–Mn–Pd are approximants of a decagonal quasicrystal with a lattice constant of 1.6 nm in the periodic direction. The unit cell of these phases contains so many atoms that the capabilities of first-principle DFT methods are exceeded by far. In order to study their structure in detail, reliable effective potentials are needed.

We have developed new analytic embedded atom method (EAM) model potentials and determined their parameters by the force-matching method. The analytic expressions are discussed. Tests with several structures will be presented.

In particular potentials for the ξ- and ξ'-phases of Al–Mn–Pd were established. Material parameters like the elastic constants were calculated. The potentials will be used to improve the structure models for the Ξ-phases and the cores of their metadislocations.

MM 7.2 Mon 10:30 H5

No miscibility gap in Pt-Rh bulk alloys — •Sascha Maisel, Tobias Kerscher, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

The phase diagram of Pt-Rh possesses an fcc-based solid solution that is stable over the whole concentration range for higher temperatures. However, for low temperatures (< 1000 K) a miscibility gap is deduced, merely from experiments on other alloys [1]. Our theoretical study comprises an ab-initio-based cluster-expansion in the framework of the UNCLE code [2]: We use input data from density-functional theory and subsequent Monte-Carlo simulations in order to account for temperature effects. Our results show that the predicted phase-separation does not occur. The resulting phase diagram will be discussed.

Supported by Deutsche Forschungsgemeinschaft

[1] B. Predel, *Landolt-Börnstein, New Series, IV/5a*, Springer 1991
[2] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009)

MM 7.3 Mon 10:45 H5

Ab-initio optimization of the crystal structure ksi and ksi* in Al- Mn-Pd — •Alejandro Santana Bonilla[1,2], Michael Engel[3], Hans-Rainer Trebin[1], and Marek Mihalkovic[4] — [1]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart — [2]Grupo de sistemas complejos, Universidad Antonio Nariño, Bogotá, Colombia — [3]University of Michigan, Ann Arbor, MI, USA — [4]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

A structural model is given for two approximants, ksi and ksi*, of the decagonal Al-Mn-Pd phase. Both structures were shown to be completely described by two sorts of interpenetrating clusters, namely *Distorted Bergman Cluster* (DBC) and by *Pseudo Mackay Cluster*(PMC). On the basis of these two atomic clusters the two phases can be characterized as some simple periodic tiling of assembly of the column clusters projected onto the plane perpendicular to the 1.6 nm stacking axis. From crystallographic studies the skeleton of heavy atoms was fully described, whereas the inner shell from PMC was poorly detailed. The structural models have been investigated using ab initio and molecular dynamics numerical methods. For this study, suitable improved pair potentials were used in order to determine the ideal cluster structure and the interactions between adjacent clusters. Plausibility of the suggested structures was tested using competing crystalline phases obtained through convex hull calculations and allowing us to suggest a reliable atomic model for the inner shell of the PMC.

MM 7.4 Mon 11:00 H5

Low temperature phases in Ni-rich Ni-W and Ni-Re — •Nils Schindzielorz, Katharina Nowak, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7, D-91058 Erlangen

It is known from experiment [1] that the mechanical properties of Ni-based superalloys heavily depend on the individual amount of W and Re in the alloy. To understand this different behaviour a detailed knowledge of the zero Kelvin groundstate diagram would be of great importance. We find, by use of a density functional theory driven cluster expansion performed with the program package UNCLE [2], that the zero Kelvin groundstate diagrams for Ni-Re and Ni-W with all possible structures based on an fcc lattice up to 20 basis atoms differ significantly. While for Ni-Re we find only one groundstate i.e. the D1a structure at 20 at.% Re, for Ni-W there are six stable groundstates with concentrations less than 40 at. % W.
Supported by Deutsche Forschungs-Gemeinschaft.
[1] H.S.Ko et al., J. Mater. Sci. **33** (1998) 3361
[2] D.Lerch et al., Modelling Simul. Mater. Sci. Eng. **17** (2009) 055003 (19pp)

MM 8: Intermetallic Phases II

Time: Monday 11:30–12:30 Location: H5

MM 8.1 Mon 11:30 H5

Perturbed γ-γ angular correlation studies of selected 211-MAX phases using ^{111}In probes — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], and Jose Mestnik-Filho[2] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil

MAX phases are nanolaminated layered carbides and nitrides, which feature an unusual set of the best attributes of both metals and high-performance ceramics. These compounds can be good electrical and thermal conductors, behave elastically stiff as well as high thermal shock resistant. To investigate the local structure of these phases, the technique of perturbed angular correlation (PAC) was used for material characterization beside x-ray diffraction and electron microscopy. Radioactive ^{111}In ions, decaying by a γ-γ cascade were implanted into the samples, sensing as *spies* their local environment via hyperfine interactions. The PAC method was applied to Nb_2InC, Ti_2AlN, Cr_2GeC and Nb_2AsC. Spectra were taken after different annealing steps to determine strength and symmetry of the electric field gradients (EFG) as a fingerprint for probe atoms on a specific lattice site and local surrounding. In each material an axial symmetric EFG was found with a characteristic quadrupole coupling constant ν_Q variing between 250 MHz and 350 MHz. Regarding to the question of lattice location of the In-probes we demonstrate that they occupy the A-site by comparing the experimental results with ab initio DFT calculations using the FP-LAPW+LO method implemented in the WIEN2k package.

MM 8.2 Mon 11:45 H5

Crack front propagation by kink formation — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

In a brittle material a travelling crack generates an upper and a lower fracture surface, which meet at a one-dimensional crack front. From a macroscopic point of view there is no reason why this curve should deviate from a straight line, contrary to the atomistic point of view, where a crack propagates by successive rupture of cohesive bonds.

We investigate fracture of the C15 $NbCr_2$ Friauf-Laves phase on an atomic level by means of molecular dynamics simulations. The numerical experiments highlight that crack fronts in general do not form a straight line and propagate by kink-pair formation at low loads (EPL 87 (2009) 66004). This mechanism should be relevant for crack propagation in any ordered brittle solid.

MM 8.3 Mon 12:00 H5

Magnetic properties of Pr_2PdSi_3 single crystals — •Yiku Xu[1,2], Fei Tang[3], Matthias Frontzek[3], Wolfgang Löser[1], Günter Behr[1], Bernd Büchner[1], and Lin Liu[2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]State Key Laboratory of Solidification Processing, Northwestern Polytechnical University,Xi'an, Shaanxi 710072, PR China — [3]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

Ternary R_2TSi_3 intermetallic compounds (R = Rare Earth, T = Transition Metal) with hexagonal AlB_2-type crystallographic structure are known because of their interesting physical properties. Pr_2PdSi_3 single crystals were grown by a vertical floating zone method. The compound exhibits congruent melting behavior at a liquidus temperature of about 1770°C. Single crystalline samples show a huge anisotropy at low temperatures due to the crystal electric field effect and order antiferromagnetically below the Néel temperature $T_N = 2.17$ K. This value approximately obeys the linear de Gennes scaling for this class of compounds. The [0 0 1] orientation was identified as the magnetic easy axis at room temperature. At lower temperature (≈ 20 K) magnetic easy and hard axes interchange with each other. Two additional magnetic phase transitions were observed at temperatures below 1 K.

MM 8.4 Mon 12:15 H5

Lattice dynamics in complex metallic alloys — •Holger Euchner[1], Marc de Boissieu[3], and Marek Mihalkovič[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Stuttgart, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia — [3]Science et Ingénierie des Matériaux et Procédés, INP Grenoble CNRS UJF, Saint Martin d'Hères Cedex, France

We report on the vibrational properties of a series of complex metallic alloys with different degrees of structural complexity.

Dynamic structure factor and vibrational density of states, obtained from inelastic X-ray and neutron scattering, are compared to both ab initio calculations and molecular dynamics simulations. This comparison is used to discuss the impact of structural complexity, as present in complex metallic alloys, on vibrational dynamics and physical properties, like specific heat and thermal conductivity.

MM 9: HV Faupel

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

Invited Talk MM 9.1 Mon 14:00 H16

Dynamic arrest in multicomponent glass forming alloys — •Franz Faupel[1], Alexander Bartsch[1], Klaus Rätzke[1], and Andreas Meyer[2] — [1]Institut für Materialwissenschaft - Materialverbunde, Technische Fakultät, Christian-Albrechts- Universität zu Kiel, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

We report radiotracer diffusivities in Pd- and Zr-based melts, presenting for the first time a complete set of data for all components over the whole relevant temperature range. While a vast decoupling of more than 4 orders of magnitude is observed between the diffusivity of Pd and of the smaller components, at the glass transition temperature T_g, the diffusivities of all components merge close to the critical temperature T_c of mode coupling theory. For Pd, the Stokes-Einstein relation holds in the whole range investigated encompassing more than 14 orders of magnitude suggesting the formation of a slow subsystem as a key to glass formation. In multicomponent Zr-based melts, dynamic heterogeneities and a slow Zr subsystem even exist in the equilibrium melt far above T_c.

MM 10: Topical Session Glass Dynamics III

Time: Monday 14:45–15:30 Location: H16

Topical Talk MM 10.1 Mon 14:45 H16

Transport Processes in Dense Melts near and far from Equilibrium — •Thomas Voigtmann — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — Zukunftskolleg, Universität Konstanz, 78457 Konstanz — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Mass transport in densely packed liquids is characterized by slow dynamical processes and a strong sensitivity of the transport coefficients to control parameters and/or external fields. I will give an overview of recent theoretical developments based on the mode-coupling theory of the glass transition and some of its nonequilibrium generalizations. I will in particular focus on the relation between tagged-particle properties as measured, e.g., through self-diffusion processes, and the collective dynamics probed for example in the inter-diffusion of concentration fluctuations in multicomponent glass formers and metallic melts. Mixtures that exhibit strong decoupling between the individual species demonstrate the similarities and differences in these processes quite clearly. Externally applied forces allow to probe the underlying dynamical processes in the nonlinear, nonequilibrium regime, and thus provide much more detailled information than just the equilibrium transport coefficients. As an example, I will discuss the relation between local, microscopic friction and its macroscopic counterpart, viscosity.

MM 10.2 Mon 15:15 H16

Structure conserving correlations, inherent structure dynamics, and the Kohlrausch-Williams-Watts behaviour of simulated metallic-glass forming Ni0.5Zr0.5 — •Helmar Teichler — Inst. f. Materialphysik, Univ. Göttingen, 37077 Göttingen, Germany

In glass forming melts near the glass temperature, the alpha-decay reflects relaxation processes with Kohlrausch-Williams-Watts behaviour on macroscopic time scales. Microscopic explanation of these fundamental features is a challenging open question, which needs understanding emergence of extreme slow dynamics with non-exponential response from atomic motions in the melt. Regarding this, we here present an analysis of microseconds-scale molecular dynamics simulation results for glass forming Ni0.5Zr0.5. The concept of "strongly effective particles" (SEPs) is used to relate the properties of macro-scale correlation functions to the atomistic processes in the melt. We show in particular that the Kohlrausch-Williams-Watts behaviour reflects structure conserving correlations (SCC) in the formation and annihilation of SEPs. The SCC make that there are long-time memory-effects in the inherent structure dynamics. Details are discussed concerning the microscopic picture behind the SCC and how to generate for relevant correlators equations of motions that take care of the SCC.

MM 11: Topical Session Glass Dynamics IV

Time: Monday 16:00–17:30 Location: H16

Topical Talk MM 11.1 Mon 16:00 H16

Slow transport in densely packed random environments — •Thomas Franosch — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany

Conventionally the dynamics close to the glass transition slowes down uniformly, deviations being often referred to as violations of the Stokes-Einstein relation. In strongly size disparate mixtures the violations may even include that only one component freezes whereas the other exhibits long-range transport often accompanied by subdiffusive motion. A minimal model explaining the observed anomalous transport is the Lorentz model where a single tracer particle meanders through a frozen array of randomly distributed obstacles. As the packing fraction of the obstacles is increased, the motion is more and more confined to narrow channels of void space accompanied with a drastic reduction of the diffusion coefficient. Contrary to the standard glass transition scenario this suppression of motion is connected to a divergent length scale characterizing the underlying geometric percolation transition of the void space. Relying on extensive computer simulation, we explain the emergence of anomalous transport, the divergence of the non-gaussian parameter, and elucidate the role of correlations in the obstacle distribution.

Topical Talk MM 11.2 Mon 16:30 H16

A structural origin of cooperativity in supercooled liquids. — •Emanuela Del Gado — ETH Zürich, Switzerland

It is still debated whether and how the onset of cooperative dynamics in supercooled liquids approaching the glass transition can take place without any straightforward connection to structural changes. We have investigated the response to static deformation of the inherent structures (IS) of supercooled liquids, by using numerical simulations of model glass formers subject to deformations, combined with local energy minimization [1]. At low temperature, where the slow cooperative dynamics arise, non-affine rearrangements of the inherent structures allow to detect the presence of large correlated domains [2]. We propose that these non-affine domains are the IS counterpart of the cooperatively rearranging regions in the dynamics, and their presence supports the connections with elastic heterogeneity found in amorphous solids. Starting from these ideas, we quantitatively study the extent of spatial correlations of non-affine rearrangements in the IS and extract a static length-scale significantly growing in the temperature range where the dynamics become strongly cooperative [3]. Our analysis indicate a new, structural signature of glass transition.

[1] H. C. Oettinger, Phys. Rev. E 74, 011113 (2006).

[2] E. Del Gado, P. Ilg, M. Kroeger and H.C. Oettinger, Phys. Rev. Lett. 101, 095501 (2008).

[3] M. Mosayebi, P. Ilg, E. Del Gado and H.C. Oettinger, in preparation.

MM 11.3 Mon 17:00 H16

Thermodynamics and kinetics of glass transition during structural ordering of Fe50Co50 — •Shuai Wei[1], Isabella Gallino[1], Ralf Busch[1], and Austen Angell[2] — [1]Department of Materials Science and Engineering, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85278, USA

The glass transition is not only the formation of an amorphous material from a supercooled liquid, but also, in general, the ergodicity-breaking of a system during a kinetic slow down process like cooling (i.e. freezing-in). Therefore, there are various kinds of glasses, conventional glasses (e.g. SiO2), spin glasses and orientational glasses...

Here we report a glass-like transition event that occurs in a simple crystalline alloy Fe50Co50 during the order-disorder transition (lambda transition). By studying the thermodynamics and kinetics of this glass-like transition, we identify the transition as a glass transition with respect to ordering of this crystalline system. The structural relaxation times as a function of temperature are fitted with the Arrhenius law and the VFT equation. The results show that the kinetics of Fe50Co50 is simple Arrhenius. We also show that the enthalpy relaxation function evolving with time is non-exponential. By comparing the glass transition of Fe50Co50 with the strong glass-formers, BeF2 and SiO2, we found that they have great similarity in heat capacity behaviour and the change in entropy. Additionally, the study solves the old problem of the incomprehensible kinks in the tail of lambda transition peak in the heat capacity curves of of β-brass and Cu3Au.

MM 11.4 Mon 17:15 H16

Proton dynamics in sodium silicate melts studied with high temperature high pressure QENS — •Fan Yang[1], Andreas Meyer[1], Tobias Unruh[2], and Eugene Mamontov[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TU München, 85748 Garching, Germany — [3]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6475, USA

We apply quasielastic neutron scattering method under high temperature high pressure condition to investigate water dynamics in hydrous silicate melts. Neutron scattering offers the possibility to access pure proton dynamics via contrast variation by isotope substitution and to understand the water transport mechanisms in great detail. With the results from the time-of-flight spectrometer TOFTOF at FRM II in combination with the ones from the backscattering spectrometer BASIS at SNS, we are able to access a microscopic dynamic time window from 0.2 picosecond up to of about 800 picoseconds. Experiments on hydrous sodium silicate melts with 10 mol% (total) water concentration have been performed at 4 different temperatures under a constant pressure of 200 MPa. Our results show that the proton dynamics in hydrous silicate melts can be fitted into a glass-glass transition scenario under the frame work of the mode coupling theory.

MM 12: Topical Session Designing Innovative Structural Materials and Steels III

Time: Monday 14:45–15:45 Location: H4

MM 12.1 Mon 14:45 H4

First principles study of thermodynamic, structural and elastic properties of eutectic Ti-Fe alloys — •Li-Fang Zhu, Alexey Dick, Tilmann Hickel, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf, Germany

Ti-based alloys have been suggested for commercial applications with a great potential due to their high strength and good corrosion resistance. The strength of these materials can be even further increased if bulk nano-structured eutectic alloys are produced. Motivated by experimental results showing eutectic Fe-Ti alloys decomposing into the FeTi compound with B2 structure and β-Ti alloys with varying Ti concentration, Ti-Fe alloys covering a broad range of Ti concentrations were studied using density functional theory within generalized gradient approximation. Our formation energies correctly predict the experimentally observed phases and we explain their stability in terms of a sensitive concentration dependence of the density of states at the Fermi level. Further, single-crystalline elastic constants as well as polycrystalline moduli are predicted employing Hershey's homogenization. Based on these results we discuss the effect of local lattice strain on the thermodynamic phase stability and elastic properties in nano-structured eutectics.

MM 12.2 Mon 15:00 H4

Importance of magnetic effects on structural properties in Al- and Si- substituted Laves phases Fe_2Nb and Fe_2W — •François Liot, Martin Friák, and Jörg Neugebauer — Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Laves phases are promising candidates for the design of new steels with superior mechanical strength. Here we study systematically thermodynamic, structural and magnetic properties in Al- and Si- substituted Laves phase compounds Fe_2Nb and Fe_2W using first-principles density functional methods. Spin polarized calculations predict that substituting Al atoms for Fe atoms in Fe_2Nb is energetically more favorable than substituting Al atoms for Nb atoms. Furthermore, they show that this leads to a significant increase of the lattice constant along the a axis. To investigate the effects of magnetism, non-magnetic calculations are carried out for the same Fe-Nb-Al compounds. Our results show that the inclusion of magnetism is crucial to accurately reproduce experimental data. Based on this insight, theoretical predictions for ternary alloys Fe-Nb-Si, Fe-W-Al and Fe-W-Si are presented.

MM 12.3 Mon 15:15 H4

The influence of interstitial carbon and substitutional Nb-Mo on the mechanical properties of Ti-Al - an ab initio study — •Dominik Legut[1,2], Juergen Spitaler[1,2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Leoben, Austria — [2]Materials Center Leoben, Leoben, Austria

Ti-Al based alloys exhibit very attractive properties such as low density, high strength at high temperatures, and very good oxidation resistance, but they are brittle at room temperature. Addition of transition elements or elements like carbon, nitrogen and oxygen can significantly improve their behavior regarding strength and ductility. We perform first-principles calculations based on density functional theory to investigate the influence of interstitial carbon on the energetics of both, the α_2 ($L1_0$) and γ (DO_{19}) structure of this alloy. The elastic constants of Ti-Al alloys with interstitial carbon are calculated and compared to the results for the pure α_2 and γ Ti-Al phases. Moreover, we study the quaternary system Ti-Al-Nb-Mo, where we determine the positions of Nb and Mo with respect to each other. Also the heat of formation is predicted for Nb-Mo concentrations which resemble the real alloy compositions.

MM 12.4 Mon 15:30 H4

Atomistic studies of dislocations in α-iron using bond-order potential — •Matous Mrovec[1,2], Christian Elsässer[1,2], and Peter Gumbsch[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]IZBS, Universität Karlsruhe, Karlsruhe, Germany

Macroscopic plastic behavior is closely linked to properties of dislocations at the nanometer scale. Direct experimental observations of the dislocation core region and of its changes during dislocation motion are unfortunately impossible and better understanding of these phenomena can be obtained only with the help of atomistic simulations. Recent atomistic studies of dislocations in iron have provided however very different outcomes, both in terms of atomic structures and energetics. The most likely reason of these large differences is a lack of reliable interatomic potentials, which would be able to describe adequately the atomic bonding and magnetic interactions in iron.

In the present work we present studies of dislocations in α-iron using a bond-order potential, which is based on a tight-binding bond representation. The model is able to capture the directional character of bonds present in transition metals and includes a description of magnetic effects within the Stoner model of itinerant magnetism. We will compare results of our simulations with available first-principles predictions as well as with predictions of other empirical interatomic potentials and discuss underlying causes of the differences.

MM 13: Topical Session Designing Innovative Structural Materials and Steels IV

Time: Monday 16:00–17:45 Location: H4

MM 13.1 Mon 16:00 H4

Atomic-scale quantification of the mechanisms underlying solid solution hardening — •Johann von Pezold, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Strasse 1, 40237 Düsseldorf

The increase in the initial flow stress of metals by the introduction of impurity atoms (solid solution hardening) is generally accounted for by a combination of the size (parelastic) and elastic (dielastic) mismatch between the host and the solute atoms. In this study we have investigated the mobility of edge dislocations in aluminum in the presence of impurity atoms using Molecular Dynamics (MD) simulations in order to quantify the relative contributions of the two effects. The Al host was described by an embedded-atom-type potential (EAM), while the impurity atoms were introduced by overlaying the EAM potential with a Lennard-Jones potential on the impurity sites, which allowed us to independently vary the size- and elastic mismatch between the metal host and the defect atoms. Our results suggest that the size mismatch is the predominant contribution to solid solution hardening, while the dielastic interaction is only of secondary importance. Based on this insight we discuss a multiscale approach for the determination of optimum hardening conditions from ab initio calculations.

MM 13.2 Mon 16:15 H4

Stability and mobility of hydrogen in the vicinity of point and extended defects in bcc-Fe — •Jutta Rogal, Yaojun A. Du, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The detrimental effect of hydrogen on materials properties poses problems for many applications. Hydrogen embrittlement of iron and steels has been studied extensively in experiments and theory, but due to the complexity of the problem it is still not fully understood. Two of the most discussed mechanisms for hydrogen embrittlement are the HEDE and HELP mechanisms. To address these mechanisms from a microscopic point of view it is important to obtain a detailed understanding of the stability and mobility of hydrogen in the vicinity of point and extended defects.

We have performed density-functional theory calculations to investigate the solubility and diffusion behaviour of hydrogen close to grain boundaries and vacancies in bcc-Fe. In bcc-Fe, hydrogen at a grain boundary is energetically favoured compared to the bulk region. Together with the very low diffusion barriers of hydrogen in bcc-Fe this may lead to a local accumulation of hydrogen around the defect even for rather small H concentrations. Employing kinetic simulations we investigate the diffusion of hydrogen in the presence of a defect and analyse the time evolution of the local hydrogen distribution.

MM 13.3 Mon 16:30 H4

In-situ investigation of precipitation in AA7449 friction stir welds using high energy SAXS — •Torben Fischer, Peter Staron, Luciano Bergmann, Jorge F. dos Santos, and Andreas Schreyer — GKSS Research Centre, Institute of Materials Research, Max-Planck-Strasse 1, 21502 Geesthacht, Germany

Friction stir welding (FSW) has in a very short time found a multitude of applications for high-tech applications in the transportation and energy industries. When engineering metallic materials are friction stir welded, thermo-mechanical processes alter the base metal microstructure and properties. The result is the formation of non-equilibrium microstructures in the joint region, which are significantly different from those found in the base material. Such non-equilibrium phases can reduce strength and toughness of the material and are normally compensated by increasing the dimensions or design complexity of integral structures.

The intermediate stages of precipitation or phase transformations in the weld zone during welding can only be registered by in-situ experiments. Therefore, a new transportable FSW system 'FlexiStir', for in-situ measurements was developed by GKSS. The in-situ experiments with the FlexiStir took place at the GKSS high-energy synchrotron beamline HARWI II at HASYLAB. Small-angle X-ray scattering (SAXS) at high photon energies was used to obtain spatial resolved results on volume fractions and sizes of precipitates at different locations in the weld zone.

MM 13.4 Mon 16:45 H4

Phase-contrast imaging with an x-ray grating interferometer in materials science using noncoherent synchrotron radiation — •Julia Herzen[1], Felix Beckmann[1], Tilman Donath[2], Malte Ogurreck[1], Stefan Riekehr[1], Christian David[2], Franz Pfeiffer[3], Astrid Haibel[1], and Andreas Schreyer[1] — [1]GKSS Research Centre, Geesthacht, Germany — [2]Paul Scherrer Institute, Villigen PSI, Switzerland — [3]Technische Universität München, Munich, Germany

Phase-contrast imaging with a hard x-ray grating interferometer is used to increase contrast for weak absorbing materials. It is a well established imaging method to visualize soft tissue in many medical and biological applications. Here we present the approach of using this method in the field of materials science, especially in imaging of new light-weight materials like magnesium and aluminium alloys. We show that more information from a single x-ray projection image can be gained by combining the different contrasts obtained by this imaging method simultaneously. This information can be used to optimize advanced joining techniques for such materials.

MM 13.5 Mon 17:00 H4

Metastable phase formation in undercooled Fe-Cr-Ni alloy melts — Thomas Volkmann[1], Wolfgang Löser[2], and •Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), D-51170 Köln — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), D-01171 Dresden

The solidification behaviour of undercooled Fe69Cr31-xNix melts, which represents the basis for the technically important stainless steels, was investigated in a wide composition range (7 at.% $<$ x $<$ 22 at.%) with respect to the competitive formation of ferrite (bcc) and austenite (fcc). The electromagnetic levitation technique was used for undercooling of bulk samples. The primary solidifying phase was identified by the analysis of time-resolved recalescence profiles that were detected by a fast responding photo diode at a rate of 1 MHz. Under equilibrium conditions the solidification mode changes from ferrite to austenite if the atomic fraction ratio of Ni/Cr = 0.5 is exceeded. It is shown that crystallization of bcc phase is preferred even at compositions where bcc is metastable. With rising undercooling a transition from primary fcc to primary bcc solidification occurs at a critical undercooling. The experimental results are compared to the predictions of the classical nucleation theory and an improved theory taking into account a finite thickness of the interface between the nucleus and the undercooled melt.

The financial support from the Deutsche Forschungsgemeinschaft under contract no. He 1601/3 is gratefully acknowledged.

MM 13.6 Mon 17:15 H4

***Ab initio* molecular dynamics study of interface layer formation at aluminum oxide/silicon nitride interfaces** — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

Ab initio molecular dynamics techniques are a powerful tool for the study of dynamic effects in materials such as vibrational properties as well as structural phase transitions and phase formations.

We present results from molecular dynamics studies of aluminum oxide/silicon nitride interfaces at elevated temperatures. The formation of new interface layers and diffusion properties are discussed.

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 13.7 Mon 17:30 H4

Ab-initio study of structural stability of Fe-B phases — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Boron is added to steels in small concentrations to improve strength, creep resistance and corrosion properties. However, the impact of boron can be beneficial or detrimental, depending on the steel composition, the boron concentration and the fabrication process itself. A conclusive picture of borons' influence on the mechanical properties and operational characteristics of steel is still missing. A first step

towards an atomistic understanding of boron in steels is the study of structural stability of Fe-B bulk phases.
To this end, we performed spin-polarized density-functional theory (DFT) calculations of the Fe-B system. In particular, we calculated the heat-of-formation of Fe-B for a large set of structures. The set of investigated crystal structures is based on a collection of experimentally observed phases of transition metals with light elements. We compare our DFT results to the experimental phase diagram of Fe-B and discuss the interaction of boron in iron.

MM 14: Diffusion and Point Defects III

Time: Monday 14:45–15:45 Location: H6

MM 14.1 Mon 14:45 H6

Atomic Study of Pipe Diffusion in Al and AlCu alloys — Jan-Michael Albina[2], Christian Elsässer[2], •Thomas Gnielka[2], and Peter Gumbsch[1,2] — [1]izbs, Karlsruher Institut für Technologie , Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

The formation energies of vacancies and activation energies for vacancy diffusion in the core of an edge dislocation in Al are investigated by means of atomistic simulations. With the climbing image nudged elastic band method it is possible to find exact saddle points for a diffusion path. The calculated formation energy for a vacancy at the core of an edge dislocation ($E_{f,v} = 0.51\ eV$) is in agreement with already published data. For the important migration step we found however a higher value of $E_{mig} = 0.43\ eV$. Based on the path of minimal activation energies, a model for the quasi 1-D diffusion will be presented.

Furthermore the influence of Cu impurity atoms on activation energies will be shown.

MM 14.2 Mon 15:00 H6

Computing ab initio free energy contributions of point defects — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Düsseldorf, Deutschland

A common assumption when computing defect concentrations is that the dominant entropy contribution is due to configurational entropy. Other entropy contributions such as harmonic and anharmonic lattice vibrations are assumed to be second order effects and are computationally expensive to calculate. Thus, such contributions have been rarely considered in defect calculations. With the increasing capability of ab initio approaches to e.g. provide accurate free energies to macroscopic approaches (e.g. CALPHAD), the inclusion of the aforementioned smaller entropy contributions will become more and more important. We have therefore developed a hierarchical scheme to coarse grain the configurations space allowing to efficiently calculate harmonic and anharmonic contributions to vacancy formation [PRB 79, 134106 (2009)]. In the present talk we will discuss the application of this approach to vacancies in aluminum and show that the inclusion of anharmonic contributions has a dramatic effect on the entropy of vacancy formation.

MM 14.3 Mon 15:15 H6

Vacancies in aluminium and dilute Al alloys - an investigation by positron annihilation spectroscopy — •Meng Liu, Benedikt Klobes, and Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn

Aluminium and its alloys are widely applied in our daily lives as construction material, food packages and so on due to their unique properties, namely light weight and high strength. In case of age-hardenable Al alloys used e.g. in automotive and aviation industry they are greatly influenced by precipitates which are usually formed through vacancy driven diffusion. In Al alloys quenched-in vacancies will be trapped by solute atoms, but in pure aluminium they diffuse to the surface, grain boundaries, dislocations and disappear at room temperature. In this study HCl solution cooled to 203 K is used instead of water as quenching medium in order to optimize quenching rate, and to freeze vacancies at such temperature. Based on this quenching method a vacancy reference in pure aluminium is obtained by using positron annihilation techniques, which are especially suitable for the investigation of open volume defects, since positrons are highly sensitive to vacancies. The results are then compared to dilute Al alloys. In this way information about solute concentration around vacancies and/or their relaxation can be obtained.

MM 14.4 Mon 15:30 H6

Comperative study of diffusion in *n*-type TCO materials — •Péter Ágoston and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, 64287 Darmstadt

In this contribution we present first-principles calculations on atomic migration for several *n*-type transparent conducting oxide (TCO) materials. We focus on the migration in the typical TCO materials In_2O_3 SnO_2, ZnO, CdO and Ga_2O_3. We have conducted total energy calculations within the framework of density-functional theory on a local level and in conjunction with the nudged elastic band method to obtain the formation and migration energies for all relevant defects in several charge states. We observe pronounced differences in the diffusion behavior for the investigated materials. This is partly caused by the different defect equilibria present in the different materials but also connected to the crystal structures and the resulting geometries of the migration processes.

MM 15: Interfaces I

Time: Monday 14:45–16:00 Location: H5

MM 15.1 Mon 14:45 H5

Ab initio characterisation of the mechanical behavior of grain boundaries — Naveed Ahmed, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, 44780 Bochum

Multiscale modeling of polycrystals requires knowledge of the elastic and plastic properties of the interfaces in their microstructure. To capture the physics of grain boundary sliding, migration, and decohesion, these processes should be investigated by atomistic calculations. Especially if the influence of segregated impurities, which can alter the bond character, shall also be described, a quantum mechanical treatment is necessary. However, the construction of continuum constitutive laws for grain boundaries from the results of ab initio calculations still requires sampling a five parameter space: the orientation of the grain boundary plane, the misorientation axis and the misorientation angle. This remains a formidable task, even with today's computers. In this paper we will introduce our investigation of the mechanical properties of grain boundaries in aluminum, which aims at replacing such a comprehensive sampling by as few representative calculations as possible. On the one hand we are investigating discriminating features in the elastic and plastic response of tilt and twist grain boundaries. On the other hand we are looking for common behavior that enables a unified treatment and a separation of variables.

MM 15.2 Mon 15:00 H5

Non-equilibrium grain boundary segregation of phosphorus in nickel-base superalloy — Lei Zheng[1] and •Tingdong Xu[2] — [1]Institute for materialphysics, university of Muenster, wilhelm-klemm-str. 10, 48149, Muenster, Germany — [2]Superalloy department, Central iron and steel research institute, xueyuan nanlu 76, 100081, Beijing, China

Applying Auger electron spectroscopy, the levels of grain-boundary segregation of phosphorus in a Ni-based superalloy are measured after solution treatment at 1200 °C for 9.8 h or at 1020 °C for 68.5 h and subsequent aging at 720 °C for 2 h. It is found that the levels of segregation increase with the solution treatment temperature. The measurement results are interpreted by the laws of equilibrium and non-equilibrium segregation. Based on this analysis, the concept of non-equilibrium grain-boundary segregation of phosphorus in a superalloy is confirmed for the first time.

MM 15.3 Mon 15:15 H5

Line stress of step edges — •Weina Li[1,2], Huiling Duan[2], and Jörg Weissmüller[1,3] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Peking University, Beijing, P.R.China — [3]Universität des Saarlandes, Saarbrücken, Germany

It is well known that the surface of a solid interact with the underlying volume phase by a mechanical force, which is quantified by the surface stress. By analogy, the line elements at solid surfaces, such as triple lines, edges, or steps may also interact mechanically with the bulk. The forces originating from lines may be derived by taking the derivative of the line tension - an excess in energy per line length - with respect to the strain. The resulting 'line stress', **t**, has not been systematically investigated so far. Consider of dimensionality, line stress should be represented by a scalar describing the magnitude of a stress directed along the line. However, it's well known that parallel step edges at planar surfaces interact via stress fields in the substrate that are dominated by normal stress components. The standard (dipole-) models [1] of step stress predict that line stress is zero. We present molecular statics computations of vicinal surfaces that show a nonzero value, with parallel and normal components. We also present a continuum model which explains the observations in terms of the extra surface stress at the inclined (up- or down-) face of the step edge. The assistance by Karsten Albe in setting up the numerical simulation is greatly acknowledged.

[1] P. Müller, A. Saul, Sur. Sci. Rep 54 (2004), 157.

MM 15.4 Mon 15:30 H5

Interfacial properties of metallic systems from molecular dynamics simulation — •Jürgen Horbach and Roberto E. Rozas — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Using molecular dynamics (MD) computer simulation, interfacial properties of crystal-liquid interfaces are investigated for the one-component metallic systems Ni and Ti. The interactions between the atoms in these systems are modeled by potentials of the embedded atom type (EAM). Inhomogeneous systems are simulated where the crystal phase in the middle of an elongated simulation box is surrounded by the liquid phase and separated by two interfaces (due to periodic boundary conditions in all Cartesian directions). The melting temperature and crystal growth coefficients are determined. At coexistence, we demonstrate how one can accurately obtain interfacial free energies from a detailed analysis in the framework of capillary wave theory.

MM 15.5 Mon 15:45 H5

Ordering dynamics of snow under isothermal conditions — •Henning Löwe, Johanna Spiegel, and Martin Schneebeli — WSL Institute for Snow and Avalanche Research SLF, Davos, Switzerland

We have investigated the morphological evolution of laboratory snow at different temperatures by means of X-ray tomography. The collective dynamics of the bicontinuous ice-vapor system is monitored by the evolution of the two-point correlation function $C(\mathbf{r}, t)$ and an ice thickness distribution. We observe the absence of dynamic scaling and reveal fundamentally different classes of length scales: The first class comprises the mean ice thickness and the ice volume per surface area. Both follow a power law $l \sim t^{1/z}$ in time, where $z \approx 3$ is in accordance with coarsening of a locally conserved order parameter. A second class of length scales is defined by the inverse partial derivatives of $C(\mathbf{r}, t)$ at the origin. The second class shows a slower growth with anomalous power law scaling $z \approx 5$. The two different power laws are consistent with fractal coarsening and reveals the persistence of long-range correlations from initial, dendritic conditions. A third class of length scales is defined by the first zero crossing of $C(\mathbf{r}, t)$ on the coordinates axes which display a non-monotonic evolution with a strong anisotropy between vertical and horizontal directions. We attribute this behavior to larger scale structural relaxations of the ice network which apparently leave the small scale, interfacial relaxations unaffected. However, vice versa it poses the question how structural mobility is induced by coarsening.

MM 16: Interfaces II

Time: Monday 16:15–17:00 Location: H5

MM 16.1 Mon 16:15 H5

Novel molecular dynamics potential for hybride metal-carbon systems — •Leonhard Mayrhofer and Michael Moseler — Fraunhofer IWM, Wöhlerstrasse 11, 79108 Freiburg

Nanomaterials based on sp^2-hybridized carbon like graphene and carbon nanotubes are objects of intense study due to their high potential for applications and their unique physical properties. But in most cases not pure all-carbon systems are of interest. E.g. for electronic or catalytic applications the carbon systems will generally be combined with metals. Therefore the aim of our work is an improved atomistic modelling of the interfaces in hybride carbon-metal-systems.

So far pair potentials are frequently used to model the interaction between carbon and metal atoms in molecular dynamics (MD) simulations [1-3]. However, this approach cannot be conciled with ab-initio calculations of various metal clusters (e.g. Al,Pd) on graphene showing a significant dependence of the metal-carbon bonding strength on the metal coordination.

We present a MD-potential in the spirit of the embedded atom method [4] giving a unified description of metal-carbon and metal-metal interactions capable of treating different metal coordinations at the same time. We apply this potential to determine realistic structures of contacts between metals and carbon nanosystems.

[1] S.Duffe et al., Euro. Phys. J. D **45**, 401 (2007)

[2] W.Y. Choi et al., Phys. Rev. B **68**, 193405 (2003).

[3] S.K.R.S. Sankaranarayanan et al., Phys. Rev. B **72**, 195405 (2005).

MM 16.2 Mon 16:30 H5

Finite element calculations of surface enhancement in attenuated total reflection infrared spectroscopy — •Ganesh Vasan and Andreas Erbe — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Surface Enhanced Infrared Absorption Spectroscopy (SEIRAS) is an effective tool at studying organic molecules in contact with metal nanostructures. Roughness or tailored structures on metal surfaces give rise to surface enhancements in the absorption spectra. A finite-element based solver of the Maxwell equations was used to simulate full spectra of organic molecules in contact with spherical and cylindrical nanostructures in the Attenuated Total Reflection (ATR) geometry on silicon internal reflection elements. Surface enhancement factors are defined, as obtained through reference runs.

The simulated field images and the absorption spectra show enhancements in both isolated and periodic cases with the absorbance increasing with decreasing inter-particle spacing. The computations confirm the experimental evidence that closer particles yield larger enhancements. Effects due to particle size have also been analysed, where larger particles show larger enhancements. The field images suggest the enhancement is because the particles act as local cavities.

MM 16.3 Mon 16:45 H5

Dielectric anti-reflective coatings for attenuated total reflection spectroscopy through metal films
— •Martina Reithmeier and Andreas Erbe —
MPI für Eisenforschung, Düsseldorf, Deutschland

In order to obtain insight into structural transformation during an electrochemical reaction, attenuated total reflection (ATR) infrared spectroscopy has proven to be a useful tool. The applicability is, however, limited when applied on continuous metal films, because of the

metal's high reflectivity. In order to overcome this limitation, we introduce a novel system of stratifications. On the incidence media (silicon, calcium fluoride or zinc selenide), a thin layer of germanium with a thickness ∼1 μm is evaporated, followed by a 20 nm gold layer.
For certain wave numbers the reflectivity of the system is significantly lowered compared to a reference system. Calculations show that a higher absorption of the investigated material is expected at these wavenumbers. Experiments based on calculations were performed on Si-Ge-Au-H_2O, CaF_2-Ge-Au-acetonitrile and ZnSe-Ge-Au-acetonitrile and -acetone systems. In acetonitrile, a splitting of most vibrational absorptions is observed in contact with gold, which could originate from the strong interaction with gold.
The experiments so far show qualitative agreement with the computations. The regions with lower reflectivity are found and can be modelled. They show a strong sensitivity towards the presence of material close to the interface. Current problems are holes in the 20 nm Au film, which have been observed by scanning electron microscopy.

MM 17: HV Schmitz

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

Invited Talk MM 17.1 Tue 9:30 H16
Interfaces in nanostructured matter — •Guido Schmitz — Inst. für Materialphysik, WWU Münster

Nanostructured materials naturally comprise interfaces in high density, reason enough to investigate their chemical structure in detail. The talk considers the impact of interfaces to stability and reaction of nanostructures. What is the natural thickness of interphase boundaries, how do new reaction products nucleate and grow at interfaces, what is the effect of interfacial curvature in core-shell nanospheres?

To answer these questions from an experimental point of view, state-of-the-art atom probe tomography is performed. Based on laser-assisted field evaporation of single atoms, this technique delivers chemical maps of outstanding spatial resolution. Due to its real 3D information, it is especially suited to the investigation of complex morphologies distinguished by curved and rough interfaces.

Based on nano-analysis of thin films and multilayers, it is shown (i) that the natural width of interfaces and its temperature dependence can be made responsible for the degradation of giant magnetoresistivity, (ii) that grain boundary transport may appear heterogeneously along 1D pipe structures, (iii) that nucleation of product phases at interfaces requires a preceding mixing on the length scale of a few nanometers, and (iv) that the reaction of spherical core-shell nanostructures may depend on the layer stacking sequence with respect to interfacial curvature.

MM 18: Topical Session Glass Dynamics V

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

Topical Talk MM 18.1 Tue 10:15 H16
The low-frequency vibrational properties of model bulk metallic glasses within the harmonic approximation. — •Peter Derlet[1], Robert Maass[2], and Jörg Löffler[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland — [2]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland

Bulk Metallic Glasses (BMGs) exhibit a rich variety of vibrational properties resulting from the significant topological disorder which occurs at the atomic scale. In the low-frequency regime confined resonant vibrational modes occur that manifest themselves as a Bose peak in the vibrational density of states. However, the precise nature of these modes and how they are influenced by local atomic structure remains unclear. Using standard harmonic analysis, this study investigates various aspects of the problem by diagonalising the Hessian of atomistic BMG structures derived from molecular dynamics simulations via a binary Lennard Jones pair potential. The results are discussed in terms of their possible relation to atomic transition pathways that result in local shear deformation zones - the underlying microscopic process contributing to the plasticity of BMGs.

MM 18.2 Tue 10:45 H16
Relaxation processes in metallic glasses studied by mechanical spectroscopy — •Dennis Bedorf, Moritz Schwabe, Stefan Küchemann, Hannes Wagner, Walter Arnold, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We are interested in understanding fundamental relaxation process in glasses, especially in metallic glasses. The use of different mechanical spectroscopy techniques enables us to get an insight of the relaxation processes with a broad range of frequencies. It is also possible to compare the relaxation behavior of samples with length scales from cm down to nm. Annealing experiments reveal reversible relaxations in bulk samples for a temperature regime, where only the β-process is commonly observed [1]. Relevant length scales of dynamic heterogeneities can be obtained from measurements under reduced sample sizes or with local probing techniques. Mechanical loss measurements of thin films indicate a critical length scale of ≈ 30 nm for the activation of slow β-processes, while local probing, using an atomic force acoustic microscope (AFAM), demonstrates the heterogeneity of the local indentation modulus.

[1] A. Kahl, T. Koeppe, D. Bedorf, R. Richert, M. L. Lind, M. D. Demetriou, W. L. Johnson, W. Arnold, and K. Samwer, APL, 95, 201903 (2009)

MM 18.3 Tue 11:00 H16
Enthalpy and free volume relaxation in a Zr-Ti-Ni-Cu-Be bulk metallic glass alloy — •Zach Evenson and Ralf Busch — Chair of Metallic Materials, Saarland University, PO Box 151150, 66041 Saarbruecken, Germany

We report on the enthalpy and free volume relaxation kinetics of the $Zr_{44}Ti_{11}Ni_{10}Cu_{10}Be_{25}$ (Vitreloy 1b) bulk metallic glass as measured with dilatometric and calorimetric methods. Using Differential Scanning Calorimetry (DSC) samples are relaxed into the metastable equilibrium liquid at temperatures below the calorimetric glass transition (T_g); the resulting enthalpy recovery ($\Delta H^{recov.}$) is then measured upon re-heating into the supercooled liquid region. It is found that the sample volume also relaxes into a metastable equilibrium liquid state, observed on a long time scale. These volumetric changes are measured isothermally using Thermal Mechanical Analysis (TMA). The total changes in the free volume ($\Delta v_f/v_m$) from the initially glassy state and the equilibrium liquid are calculated during annealing at the same temperatures as in DSC. The equilibrium free volume change is found to relax with a stretched exponential behavior and is best fitted with a Kohlrausch-Williams-Watts (KWW) function with beta-values approaching unity close to the glass transition. The measured values of $\Delta H^{recov.}$ and $\Delta v_f/v_m$ correlate well within the framework of free volume theory and a linear relationship is found between the two.

MM 19: Topical Session Designing Innovative Structural Materials and Steels V

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

Topical Talk MM 19.1 Tue 10:15 H4

Influence of pressure on decomposition thermodynamics of structural materials — •Igor A. Abrikosov[1], Björn Alling[1], Alena V. Ponomareva[2], Olga Yu. Vekilova[1], and Sergei I. Simak[1] — [1]Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden — [2]Department of Theoretical Physics, Moscow State Institute of Steel and Alloys, Moscow 119049, Russia

We show, by means of state-of-the-art theoretical simulations, that a pressure which is often present in practical applications of structural materials may have profound effect on their decomposition thermodynamics. In TiAlN, which is widely used as hard protective coating in cutting tool applications, the hydrostatic pressure enhances the tendency for isostructural decomposition, including spinodal decomposition. In Fe-Cr steels we observe a concentration reversal of pressure induced tendency towards isostructural decomposition.

Topical Talk MM 19.2 Tue 10:45 H4

Computational Phase Studies: Deriving thermodynamic properties of metals from first principles — •Tilmann Hickel — MPI für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf

In the past few years the combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic concepts has so quickly advanced, that they now allow tackling even complex engineering systems such as steels, shape-memory alloys or light-weight metals. The key for a reliable predicting also phase transitions is the availability of efficient and highly accurate theoretical tools to determine free energies from ab initio. We have therefore performed an extensive and systematic study of the capabilities of present day implementations (xc-functionals) of densitiy functional theory in determining ab initio free energies for metals. Lattice vibrations, which yield the dominant contribution to the free energy of elementary, non-magnetic materials, can be determined within the quasiharmonic approximation. We were able to show for a large set of metals that the thus derived thermodynamic properties are in excellent agreement with available experimental data. For magnetic materials such as iron we have developed a proper quantum-mechanical treatment of magnetic excitation, improving previous classical approaches. An integrated approach, combining electronic, vibrational, and magnetic effects, lead us to an extremely high accuracy of only a few meV for the free energy of the considered metals. The thus determined free energies have been successfully used to predict martensitic phase transition temperatures in selected materials such as shape memory alloys.

MM 20: Topical Session Designing Innovative Structural Materials and Steels VI

Time: Tuesday 11:30–13:00 Location: H4

MM 20.1 Tue 11:30 H4

Ab initio analysis of the carbon solubility limits in various iron allotropes — Olga Kim, •Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

The solubility limits of carbon in various iron phases are of critical importance for many steel-industry applications. The actual values are difficult to measure accurately in ferrite and they have so far not be determined theoretically from first principles in austenite. The solubility limits of carbon in α, β, γ, and δ iron have been thus determined employing density functional theory calculations over the entire temperature range. The results show excellent agreement with experiment. The two-orders-of-magnitude higher solubility of carbon in austenite than in ferrite has been quantitatively analyzed and a complex interplay between two distinct phenomena has been found. First, the number of first nearest neighbors is higher in the fcc structure than in the bcc structure and the carbon atom is consequently more strongly bound, and secondly, the strain energy between the C-interstitial and the surrounding iron matrix is lower in the fcc lattice. The details of the actual magnetic state have not been found as important as the above mentioned two mechanisms.

MM 20.2 Tue 11:45 H4

Multi-scale study of martensite stability in Fe-based solid solutions — •Alexander Udyansky, Johann von Pezold, Aleksey Dick, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

Martensitic phases refer to tetragonal states of interstitial solid solutions. We study such Fe-based dilute phases by combining atomistic modeling with the reciprocal space microscopic elasticity theory (MET), which allows us to account for long-ranged elastic interactions between impurities. The short-range chemical interactions, as well as the parameters entering the MET are obtained by density functional theory (DFT) calculations. This approach allowed us to compute temperature/interstitial concentration phase diagrams and provided a direct insight into the stability limits and formation mechanisms of martensite: specifically, tetragonal states are predicted to be preferred even at low impurity concentrations of carbon, nitrogen and oxygen due to a thermodynamically driven orientational ordering of the interstitials. Moreover, both the structural type of the tetragonal state and the transition temperature were found to sensitively depend on the local strain state of the system.

MM 20.3 Tue 12:00 H4

Ordering and precipitation in Ni-rich Ni-W and Ni-Re — •Nils Schindzielorz, Katharina Nowak, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7, D-91058 Erlangen

The unusual high hardening effect of Re compared to that of W when alloying them to Ni-based superalloys has already been discussed to be caused by the formation of precipitates within the Ni matrix [1]. By the combination of a density functional theory based cluster expansion Hamiltonian with Monte-Carlo simulations using the programme package UNCLE [2] it will be shown that for Ni-Re in the dilute limit with concentrations less than 10 at. % precipitates with a D1a structure emerge within the γ phase whereas for Ni-W the dominant effect is the formation of solid solutions. The interpretation of the calculated short range order patterns clarifies these results. However, for less than 5 at. % also in Ni-W indications can be found for the formation of precipitates.

Supported by Deutsche Forschungs-Gemeinschaft.

[1] J.Rüsing et al., Scripta Materialia **46** (2002) 235-240

[2] D.Lerch et al., Modelling Simul. Mater. Sci. Eng **17** (2009) 055003 (19pp)

MM 20.4 Tue 12:15 H4

New structure maps for topologically close-packed phases in Ni-based superalloys — Bernhard Seiser[1], Thomas Hammerschmidt[2], •Ralf Drautz[2], and David G. Pettifor[1] — [1]Department of Materials, University of Oxford, Oxford, United Kingdom — [2]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Refractory elements like Re and W are added to Ni-based superalloys to improve the creep resistance. It is observed that too large concentrations induce the formation of topologically close-packed phases (TCPs) that destroy the single-crystal lattice of the Ni-based superalloys and are detrimental to the mechanical properties. In this talk we will present analytic bond-order potentials that are suitable for the prediction of TCP phase stability. By using the moments theorem that relates the crystal structure to the electronic density of states, the analytic interatomic bond-order potentials are obtained by expanding the tight-binding electronic structure in terms of response functions that depend on the Fermi energy and moments of the density of states that are given as functions of the local atomic environment. With the help of the analytic bond-order potentials the structural stability of TCP phases is then characterized as a function of valence-electron count and lattice structure. For example, at the fourth moment level we observe a distinct separation of the TCP phases in two groups. Based on the analysis of the stability of the TCP phases as a function of size difference and valence-electron count, we propose a new structure map that separates the TCP phases in different regions of stability. We compare the predictions of the structure map to DFT calculations.

MM 20.5 Tue 12:30 H4

Entropic stabilisation of topologically close-packed phases in binary transition-metal alloys — •Thomas Hammerschmidt[1], Bernhard Seiser[2], Suzana G. Fries[1], Ingo Steinbach[1], Ralf Drautz[1], and David G. Pettifor[2] — [1]ICAMS, Ruhr-Universität Bochum, Bochum, Germany — [2]Department of Materials, University of Oxford, Oxford, United Kingdom

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the mechanical 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. It is well known that the structural stability of the tcp phases A15, σ and χ is driven by the average d-band filling. For a direct comparison to experimental phase diagrams, we carried out extensive density-functional theory (DFT) calculations of the tcp phases A15, C14, C15, C36, μ, σ, and χ in tcp-forming binary transition-metal (TM) systems. We observe several systems such as W-Re with positive values of the heat of formation for all tcp phases although some of the phases are observed experimentally. By combining our DFT total energies with the CALPHAD methodology, we can demonstrate that configurational entropy can stabilise the tcp phases in these systems.

MM 20.6 Tue 12:45 H4

Anomalous thermal expansion in iron-nickel alloys: *ab initio* calculations and the relation to magnetism — •François Liot[1] and Chris Hooley[2] — [1]Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, U.K.

The thermal expansion of ferromagnetic disordered iron-nickel alloys at various temperatures is studied, using an approach based on Ising magnetism and first-principles calculations of the disordered local moment (DLM) type. The theory correctly describes the strong increase of the thermal expansion coefficient with increasing nickel concentration from 0.35 to 0.8 at room temperature. It also reproduces the Invar effect for $x = 0.35$. These results are analyzed, and the effect of the magnetic free energy contribution on the thermal expansion is discussed. Furthermore, a simple relationship between anomalous thermal expansion and magnetism is presented. It is argued that an alloy shows the Invar effect if the concentration of nearest-neighbor iron-iron pairs with anti-parallel local moments increases sufficiently rapidly with temperature over a broad temperature interval.

MM 21: Mechanical Properties I

Time: Tuesday 10:15–11:30 Location: H6

MM 21.1 Tue 10:15 H6

Plastische Verformungen und Schmelzerscheinungen beim makrospröden Bruch von Polyäthylenkörpern. — •Heinz Hans Walter Preuss — Hameln

Berichtet wird über eine bislang weitgehend unbeachtet gebliebene Entdeckung aus dem Jahre 1962 [1, 2, 3], die jünst bestätigt wurde [4]. Bei elektronenmikroskopischen Untersuchungen von Kohlenstoffabdrücken der Bruchfläche von Niederdruck-Polyäthylen-Proben waren morphologische Erscheinungen gefunden worden, wie sie nur nach dem Zerreißen einer zähflüssigen Substanz entstehen können, insbesondere Zapfen mit verdicktem abgerundeten Ende. Die Proben waren mit einer Biegevorrichtung mit Lastvorgabe bei Raumtemperatur und bei der Temperatur des flüssigen Stickstoffs gebrochen worden. Die der endgültigen Trennung vorausgehenden lokalen plastischen Deformationen führen dank der niedrigen Wärmeleitfähigkeit des Materials zur Erwärmung bis zur Schmelztemperatur (115oC), so dass die Trennung örtlich differenziert in zähflüssigen Phase erfolgt. Die ursprünglichen Abrissformen bilden sich nach der Trennung in abgerundete Formen und erstarren in der beobachteten Gestalt. Literatur: 1 H. H. W. Preuß, Plaste und Kautschuk, 10 (1963) Nr. 3, 161 2 H. H. W. Preuß, Plaste und Kautschuk, 10 (1963) Nr. 6. 330 3 H. H. W. Preuß, Dissertation, Leipzig, 1963 4 I. Brough, R. N. Haward, G. Healey, A. Wood, Polymer 45 (2004) 3115 - 3123

MM 21.2 Tue 10:30 H6

Deformation behavior of polycrystalline intermetallic compounds YAg and YCu — •Rolf Schaarschuch[1], Carl-Georg Oertel[1], Guanghui Cao[2], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Materials Engineering, Shanghai University, Shanghai 200072, P.R. China

The influence of texture on the deformation behavior of YCu and YAg, intermetallic compounds with B2 structure, was studied by compression at room temperature on hot extruded polycrystalline material. The phase constitution and texture of the materials were determined by X-ray diffraction. The texture is characterized by a weak <110> fiber along the extrusion axis. The compression with a strain rate of about $10^{-4}\mathrm{s}^{-1}$ was done parallel and perpendicular to the extrusion axis. The deformation experiments show a higher flow stress for YAg in comparison to YCu. This may be caused by a small amount of second phase YAg_2. Because of the weak fiber texture the flow stress perpendicular to the extrusion direction is slightly higher than parallel. The results are discussed with respect to the ductility of intermetallic compounds with B2 structure.

MM 21.3 Tue 10:45 H6

Dislocations in the Complex Metallic Alloy T-Al-Mn-Pd — •Marc Heggen, Lothar Houben, and Michael Feuerbacher — Institut für Festkoerperforschung, Forschungszentrum Juelich GmbH, D-52425 Juelich, Germany

The deformation mechanisms of complex metallic alloys - crystalline solids containing up to thousands of atoms per unit cell - are widely unknown. Due to the large lattice parameters of these materials, conventional dislocation mechanisms are prone to failure. We investigated the complex metallic alloy T-Al-Mn-Pd with 156 atoms per unit cell using aberration-corrected high-resolution transmission electron microscopy. We found a highly complex deformation mechanism, based on the movement of a dislocation core mediating strain and separate escort defects. Upon deformation, the escort defects move along with the dislocation core and locally transform the material structure. This mechanism implies the coordinated movement of hundreds of atoms per elementary glide step. Nevertheless it can be described by simple rearrangement of basic structural subunits.

MM 21.4 Tue 11:00 H6

Complementary Climb Systems: Deformation Mechanism in Complex Metallic Alloys — •Michael Feuerbacher, Stefan Roitsch, and Marc Heggen — Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52345 Juelich

Complex metallic alloys (CMAs) are hallmarked by a high number of atoms per unit cell and a cluster based substructure dominated by icosahedral atom coordination. Due to their large lattice parameters, conventional dislocation-based deformation mechanisms are prone to failure in these materials. In recent years we have experimentally characterized the plastic deformation mechanism of a number of CMAs. We find that in many instances, strain is mediated by dislocations moving by pure climb. In uniaxial compression experiments we find two sets of dislocations. One set is moving on planes perpendicular to the compression direction by positive climb. This leads to shortening of the sample by removal of atom planes and consumes vacancies. The second set has habit planes perpendicular to the compression direction. This set moves by negative climb and hence acts as a vacancy source for the first system. The complementary action of the two sets avoids vacancy depletion and breakdown of the plastic deformation mechanism. The measured dislocation densities lead to vacancy diffusion distances consistent with the applied deformation rates in our experiments. We demonstrate the action of this mechanism in a number of CMA phases.

MM 21.5 Tue 11:15 H6

Crack tip opening displacement and propagation rate of microstructurally short cracks in austenitic stainless steel — •Michael Scharnweber[1], Ingmar Roth[2], Martin Kübbeler[3], Carl-Georg Oertel[1], Wolfgang Tirschler[1], Hans-Jürgen Christ[2], Claus-Peter Fritzen[3], Ulrich Krupp[4], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden — [2]Institut für Werkstofftechnik, Universität Siegen, 57076 Siegen — [3]Institut für Mechanik und Regelungstechnik, Universität Siegen, 57076 Siegen — [4]Fakultät für Ingenieurwissenschaften und Informatik, Fachhochschule Osnabrück, 49009 Osnabrück

Austenitic stainless steel (X2 CrNiMo 18 14 3) has been cyclically deformed at RT in air under plastic strain control with an amplitude of $5*10^{-4}$ for N=10000 cycles to initiate microstructurally short cracks. Average crack propagation rates were measured with the scanning electron microscope (SEM) in steps of ΔN=5000 cycles. Additionally, the crack tip opening displacement (CTOD) was obtained via in-situ-deformation in the SEM. It is the aim of the present study to quantify the influence of grain boundaries on crack growth and determine the correlation between the two values measured. This may offer the possibility to replace time consuming measurements of the crack propagation rate by the much quicker measurement of the CTOD.

MM 22: Hydrogen in Metals

Time: Tuesday 10:15–11:30 Location: H5

MM 22.1 Tue 10:15 H5

First-principles and thermodynamic description of hydrogen interaction with vacancies in fcc iron — •Roman Nazarov, Tilmann Hickel, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Duesseldorf, Germany

Several mechanisms of hydrogen embrittlement are associated with a significant increase of the vacancy concentration in a H-rich atmosphere. These superabundant vacancies can form vacancies clusters or even microvoids in regions of high stress (for example crack tips), facilitate the formation of brittle phases and reduce elastic properties of crystalline structure.

In order to reveal the physics of this phenomenon we have employed density-functional theory (DFT) together with thermodynamic concepts. Our systematic comparison of isolated and hydrogen loaded vacancies in fcc iron with various magnetic configurations reveals that hydrogen reduces the formation energy of a vacancy. This decrease can be significant, as up to 6 hydrogen atoms can be incorporated into a vacancy.

Based on our ab-initio results we developed a thermodynamic model which determines the concentrations of vacancies, of hydrogen in different interstitial positions and of vacancy-hydrogen complexes as a function of pressure, temperature and external hydrogen chemical potential. Applying this model we find dramatically increased vacancy concentrations and total hydrogen concentration in fcc iron if the material is exposed to a H-rich atmosphere.

MM 22.2 Tue 10:30 H5

First-principles studies of the La-H system — Gunther Schöllhammer[1], Peter Herzig[1], Walter Wolf[2], •Tobias Kerscher[3], and Stefan Müller[3] — [1]Institut für Physikalische Chemie, Universität Wien, 1090 Wien, Austria — [2]Materials Design s.a.r.l., 72000 Le Mans, France — [3]Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

The LaH system is the epitome of an interesting candidate for theoretical investigations: Its structural details are still not well understood, and – at $LaH_{\approx 2.8}$ – a concentration-dependent metal-insulator transition (“switchable mirror”) is observed. At low H concentrations our first-principles study found a preference of the H atoms for the occupation of the octahedral interstitial sites instead of the expected tetrahedral sites. Close to LaH_3 a stabilization of the structure either by an orthorhombic distortion or by the presence of (pairs of) H vacancies was observed. This coincides with opening up a band gap predicted via density functional theory [1]. Recently we have applied the cluster-expansion approach (see e.g. [2]) in the framework of the UNCLE code [3] in order to study configurational diversity. The objective is the calculation of a phase diagram from first-principles.

[1] G. Schöllhammer, W. Wolf, P. Herzig, K. Yvon, P. Vajda, J. Alloys Comp. **480**, 111–113 (2009)

[2] S. Müller, W. Wolf, R. Podloucky, *Ab-initio Methods and Applications*, in *Alloy Physics*, ed. W. Pfeiler, Wiley 2007

[3] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009)

MM 22.3 Tue 10:45 H5

Strain-induced metal-hydrogen interactions across the first transition series: An ab initio study of hydrogen embrittlement — •Johann von Pezold, Liverios Lymperakis, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

The attractive interaction between hydrogen and distorted regions of the host matrix underlies all the currently discussed mechanisms of hydrogen-induced embrittlement of metals, such as hydrogen enhanced local plasticity (HELP), hydrogen enhanced decohesion (HEDE) and stress-induced hydride formation. In this study we investigate these interactions systematically by determining heat of solutions, H-H binding energies within the metal matrix, as well as phase diagrams as a function of the lattice strain and the H chemical potential across the first transition series (3d elements) using density functional theory (DFT) calculations. It will be shown that these provide a very direct insight and allow an identification of the likely embrittlement mechanisms within these metals.

MM 22.4 Tue 11:00 H5

Li-Al-borohydride as a potential candidate for on-board hydrogen storage — •Inge Lindemann[1], Roger Domènech Ferrer[1], Lothar Dunsch[1], Yaroslav Filinchuk[2], Hans Hagemann[3], Radovan Černý[3], Ludwig Schultz[1], and Oliver Gutfleisch[1] — [1]IFW Dresden, PO Box 270016, D-01171 Dresden, Germany — [2]Swiss-Norwegian Beam Lines at ESRF, BP-220, 38043 Grenoble, France — [3]University of Geneva, Crystallography and Physical Chemistry Department, 1211 Geneva, Switzerland

Recently, double-cation borohydride systems have attracted great interest. It was found that the desorption temperature of the borohydrides decreases with increasing electronegativity of the cation. Consequentely, it is possible to tailor a feasible on-board hydrogen storage material by combination of appropriate cations. Li-Al-borohydride shows a desorption temperature suitable for applications ($\approx 70°$C) combined with an high hydrogen density (17.2 wt.%). It was synthesised via high energy ball milling of $AlCl_3$ and $LiBH_4$. The structure of the compound was obtained from high-resolution synchrotron powder diffraction and shows a unique complex structure within the borohydrides. The material was characterized by means of in-situ-Raman, DSC, TG and thermal desorption measurements to study its decomposition pathway. The desorption at $\approx 70°$C results in the formation of $LiBH_4$ while the high mass loss of about 20% points to the release of not only hydrogen but also diborane. This is right now the main drawback for applications because it hinders reversibility.

MM 22.5 Tue 11:15 H5

Effects of recrystallization on the deuterium retention in tungsten — •Armin Manhard and Klaus Schmid — Max-Planck-Institut für Plasmaphysik, EURATOM Assoziation, Boltzmannstr. 2, 85748 Garching

Tungsten is a promising material for plasma-facing surfaces in nuclear fusion devices such as ITER. In these machines the surface material is exposed to large fluxes and fluences of hydrogen isotope ions and energetic neutrals. The retention of hydrogen isotopes in tungsten is generally considered small. The underlying mechanisms are yet only poorly understood despite continued research efforts. Especially the microstructure of the material can have a large influence on the hydrogen inventory.

To investigate this, the microstructure of tungsten samples from the same base material is systematically modified by recrystallization. After a thorough characterization by electron microscopy, strongly deformed samples and samples recrystallized by different degrees are loaded with deuterium in a low-temperature plasma device. The ion energy is adjusted by sample biasing. The deuterium inventory is then measured by nuclear reaction analysis and thermal effusion spectroscopy. The surface morphology is investigated by optical and atomic force microscopy. Microscopic markers applied to the sample surface allow to observe the identical surface region after each treatment step. The results are presented and compared for the different microstructures.

MM 23: Quasicrystals

Time: Tuesday 11:45–12:30 Location: H5

MM 23.1 Tue 11:45 H5

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

A theory of the hydrodynamic structure factor for quasicrystals is developed and exploited. Based on the hydrodynamic equations for icosahedral quasicrystals we introduce the terms of dynamic correlation and response. The phononic and phasonic diffuse part of the dynamic structure factor are examined in detail in frequency and time domain. We present a complete set of solutions for the hydrodynamic equations. Out of the diffusive modes we separately study the phasonic diffusion, the anisotropy of the phasonic diffusion constants and the general solution for phason wall diffusion. All results include phonon-phason coupling.

MM 23.2 Tue 12:00 H5

Transmission of Light in Dielectric Multilayers based on Metallic Means Sequences — •Stefanie Thiem[1,2], Michael Schreiber[1], and Uwe Grimm[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Department of Mathematics and Statistics, The Open University, Milton Keynes MK7 6AA, United Kingdom

The light propagation through a quasiperiodic stack of layers with different indices of diffraction is studied using the transfer matrix method. The layers are aligned according to metallic means sequences depending on a parameter m with an inflation rule $\mathcal{P} = \{B \rightarrow A, A \rightarrow ABA^{m-1}\}$ denoting the indices of diffraction n_A and n_B, respectively. We focus on the dependence of the light transmission on the underlying construction rule and obtain that additional transmission bands occur for frequencies corresponding to the photonic band gap of the periodic system. Further, we obtain almost complete transmission for the quasiperiodic systems for a wide range of ratios of diffractive indices n_A/n_B in contrast to systems with periodically stacked layers. In addition, our numerical results indicate that the transmission coefficient becomes either 1 or 0 for very large systems while usually for smaller approximants of the quasiperiodic systems also intermediate values of the transmission coefficient T occur. This corresponds to either complete reflection or transmission of the light for an infinite stack.

MM 23.3 Tue 12:15 H5

Binary Tilings with n-fold Symmetry — •Johannes Roth — ITAP, Universität Stuttgart

In the field of quasicrystals, binary tilings are rhombus tilings with vertices decorated alternatively with large and small atoms. Binary tilings have played an important role in computer simulations of decagonal quasicrystals, for example in the study of the properties of random tilings, dislocations, cracks and so on.

In this contribution we study the possibility to generalize the decagonal case to arbitrary rotational symmetries. Basically it is easy to show that a generalization is possible in many cases, but our purpose is to find tilings with nice properties, especially for example Bragg reflection.

MM 24: BV Matwerk

Time: Tuesday 13:30–13:45 Location: H16

MM 24.1 Tue 13:30 H16

Bundesvereinigung Materialwissenschaft und Werkstofftechnik (BV MatWerk) — •Dieter Herlach[1], Günter Gottstein[2] und Pedro Dolabella Portella[3] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Institut für Metallkunde und Metallphysik, RWTH Aachen — [3]Bundesanstalt für Materialforschung und Werkstofftechnik Berlin

Ursprünglich angeregt durch ein Votum des Wissenschaftsrats und später durch Initiative der Deutschen Forschungsgemeinschaft gründete sich am 22. Oktober 2007 die Bundesvereinigung für Materialwissenschat und Werkstofftechnik, kurz BV MatWerk. Derzeit umfasst BV MatWerk 29 Mitgliedsverbände und Arbeitskreise, die in Deutschland auf den Gebieten Materialwissenschaft und Werkstofftechnik tätig sind. Durch einstimmigen Beschluss des Vorstandsrates der Deutschen Physikalischen Gesellschaft (DPG) vom 10. November 2007 ist die DPG Mitglied von BV MatWerk. Der Fachverband Metall- und Materialphysik vertritt die DPG in der Mitgliederversammlung von BV MatWerk. Gleichzeitig wurde der damalige Sprecher des Arbeitskreises Festkörperphysik, Professor Dr. Rolf Haug in den Beirat der Bundesvereinigung berufen. Das diesjährige Tagungsprogramm der Arbeitsgemeinschaft Metall- und Materialphysik wurde gemeinsam mit BV MatWerk gestaltet. In unserem Beitrag berichten wir über die Ziele und Aktivitäten der Bundesvereinigung.

MM 25: HV Riedel

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

Invited Talk MM 25.1 Tue 14:00 H16

Models for ductile fracture and their application to forming processes — •Hermann Riedel — Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg

Models for ductile fracture of metals and alloys describe the nucleation, growth and coalescence of voids. Constitutive models, such as the classical Gurson model and its successors, include the effect of the evolving damage on the strength of the material. In the framework of the finite element method, these models are useful tools for predicting crack formation in components during forming operations or under crash conditions. Edge cracking in rolled sheets serves as an example to demonstrate the superiority of advanced compared to simpler models. Only mechanism-based models are able to reproduce the characteristic zig-zag pattern of the cracks on the side surface of the sheet. Another important aspect of ductile fracture is the necking of specimens or components and its interaction with the internal void growth.

MM 26: Poster Session

Time: Tuesday 14:45–16:30 Location: Poster C

MM 26.1 Tue 14:45 Poster C

Ultra-fast diffusion paths in nickel after ECAP — •Gerrit Reglitz, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The concept of so called "non-equilibrium" grain boundaries describes a specific (highly defected) type of grain boundaries in materials, which are produced by severe plastic deformation like ECAP (equal channel angular pressing) or high-pressure torsion. These specific grain boundaries are supposed to have a high density of extrinsic (excess) grain boundary dislocations, and, thus, higher excess grain boundary energy, larger free volume and enhanced diffusivity. To investigate the different types of grain boundaries in Ni after severe plastic deformation by ECAP the self-diffusion experiments were carried out by using the ^{63}Ni isotope in combination with a parallel sectioning technique. The results of these investigations highlight the existence of different types of grain boundaries in this material with completely unequal diffusion characteristics. The kinetic properties are dramatically affected by a preliminary heat treatment. The concept of the "non-equilibrium" grain boundaries in severely deformed materials is critically discussed on the basis of the present data. Support by DFG is gratefully acknowledged.

MM 26.2 Tue 14:45 Poster C

Individual precipitates in Al alloys probed by the Bonn Positron Microprobe — Osman Balarisi[1], Patrick Eich[1], Matz Haaks[1], Sven-Martin Hühne[2], •Benedikt Klobes[1], Björn Korff[1], Werner Mader[2], Karl Maier[1], Reinhard Sottong[1], and Torsten Staab[3] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn — [2]Institut für Anorganische Chemie , Römerstraße 164, 53117 Bonn — [3]Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg

Positron annihilation spectroscopy (PAS) is a unique tool for the charaterization of open-volume defects such as vacancies. Therefore, age hardenable Al alloys, whose decomposition is mainly driven by the vacancy mechanism of diffusion, are often charaterized by PAS techniques. Nevertheless, probing the defect state of individual precipitates grown in Al alloys requires a focused positron beam and has not been carried out up to now. In this respect we present the first investigations of the defect state of individual precipitates utilizing the Bonn Positron Microprobe (BPM). Furthermore, the analysis of the experimental data has to be facilitated by theoretical calculations of the observables of positron annihilation spectroscopy.

MM 26.3 Tue 14:45 Poster C

Comperative study of point defects in *n*-type TCO materials — •Péter Ágoston[1], Paul Erhart[2], Andreas Klein[1], Risto M. Nieminen[3], Martti J. Puska[3], and Karsten Albe[1] — [1]Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, 64287 Darmstadt — [2]Lawrence Livermore National Laboratory, L-367, Livermore, CA 94550, USA — [3]Department of Applied Physics, Helsinki University of Technology, FIN-02015 TKK, Finland

The performance of transparent conducting oxides (TCO) is strongly interrelated with their point defect thermodynamics and kinetics. In this contribution we present first-principles calculations on the point defects and their migration in typical *n*-type TCO materials. We focus on the TCO materials In_2O_3, SnO_2, ZnO, CdO and Ga_2O_3. We have conducted total energy calculations within the framework of density-functional theory on a semi-local level and in conjunction with the nudged elastic band method to obtain the formation and migration energies for all relevant defects in several charge states. The defect formation energies are corrected using the hybrid functional DFT methodology and are therefore not affected by the DFT band gap error. Within this band gap error free description we present the general trends of the point defect thermodynamics and kinetics in these materials and also point out important differences.

MM 26.4 Tue 14:45 Poster C

Atomic-Scale Modeling of Diffusion-Driven Microstructure Evolution in Irradiated Metals — •Erik Bitzek[1,2], Sanket Sarkar[3], William T. Cox[3], Thomas Lenosky[2], Yunzhi Wang[3], and Ju Li[2] — [1]Lehrstuhl Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg — [2]Department of Materials Science and Engineering, Ohio State University, Columbus, OH, USA — [3]Department of Materials Science and Engineering, School of Engineering and Applied Science, University of Pennsylvania, Philadelphia, PA, USA

Diffusion of vacancies and impurities plays an important role in irradiated materials. The elementary diffusion processes are readily studied at the atomic scale and the results can be used to compile event catalogs needed by kinetic-Monte-Carlo (kMC) simulations of diffusion. However, the interplay between diffusion and changes in the microstructure remains less well understood, as it involves not only random motion of vacancies in stress gradients but also the concerted motion of atoms, e.g. during dislocation nucleation or glide. The different time scales involved in these processes pose a general challenge to modeling approaches.

Here we present a novel computational method, termed diffusive molecular dynamics (DMD), which allows for the study of diffusion driven evolution of complex microstructures at the atomic scale. The utility of DMD to investigate processes related to irradiation damage is demonstrated by studies on void formation and growth and the creation of stacking fault tetrahedra (SFT).

MM 26.5 Tue 14:45 Poster C

Introducing variable barrier heights in Kinetic Monte-Carlo simulations: A study of order-order transitions in $L1_2$ ordered Ni_3Al based on first-principles calculations — •Martin Leitner[1], Doris Vogtenhuber[2], Wolfgang Pfeiler[1], and Wolfgang Püschl[1] — [1]University of Vienna, Faculty of Physics, Department Dynamics of Condensed Systems — [2]University of Vienna, Faculty of Physics, Department of Computational Materials Science

Kinetic Monte-Carlo (KMC) simulation is a valuable tool when it comes to studying atom jump behavior in detail, for instance the kinetics of the long-range ordered state in intermetallics which is a precondition for a lot of favorable material properties. We introduce an improved KMC algorithm with variable saddle point heights depending on atom environment. In transition state theory the barrier height is the energy difference between the initial equilibrium state and a saddle point state which was mostly set constant in traditional treatments. In contrast, taking $L1_2$ ordered Ni_3Al as a model system, an explicit calculation of the saddle point height is proposed and demonstrated. It is seen that the 4-atom window through which the jumping atom has to pass is decisive. We calculated *ab initio* a complete set of jump energy profiles for all possible jump types and window occupations. In KMC simulations we tested the influence of this explicit calculation and compared it to the old paradigm of constant saddle point heights. It turned out that individually computed saddle point energies make a considerable difference in jump statistics and overall kinetics.

MM 26.6 Tue 14:45 Poster C

Investigation of Li dynamics in gas-phase synthesized amorphous oxides by NMR and impedance spectroscopy — •Viktor Epp, Christian Brünig, Martin Wilkening, Michael Binnewies, and Paul Heitjans — Leibniz Universität Hannover, D-30167 Hannover

Currently, great effort is put into finding novel ion conductors that meet the requirements of modern energy storage systems. The characterization of their transport properties with complementary methods plays a crucial role in this research area. Here, metastable, highly non-stoichiometric oxides containing Al, Li and Si were studied by impedance spectroscopy (IS) and, complementarily, by various ^{7}Li NMR techniques which are capable to probe Li dynamics on different time and length scales [1, 2]. The samples, which are X-ray amorphous, were synthesized via a gas-phase reaction [3] from $AlCl_3$, LiCl and $SiCl_4$. The applied NMR techniques included the analysis of ^{7}Li NMR spin-alignment echoes, line shapes as well as spin-lattice relaxation (SLR) rates $T_{1\rho}^{-1}$ in the rotating frame of reference. When probed on the same time scale, good agreement is found between the activation energies obtained from IS and SLR NMR. Altogether, the Li diffusivity in the investigated oxide turned out to be rather slow.

[1] M. Wilkening, V. Epp, A. Feldhoff, P. Heitjans, J. Phys. Chem. C 112 (2008) 9291.
[2] M. Wilkening, P. Heitjans, Phys. Rev. B 77 (2008) 024311.
[3] T. Giesenberg, S. Hein, M. Binnewies, G. Kickelbick, Angew.

Chem. Int. Ed. 43 (2004) 5697.

MM 26.7 Tue 14:45 Poster C

Interplay between structural disorder and magnetic susceptibility in FeSi — •Tommy Reimann, Dirk Menzel, Dirk Schulze Grachtrup, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

The narrow gap semiconductor FeSi has been of high experimental and theoretical interest for over 60 years, mostly due to its unusual magnetic behavior. To clarify the reasons for the Curie-Weiss-like reincreasing of the magnetic susceptibility at low temperatures, we performed transport and susceptibility measurements on different FeSi single crystals grown via the tri-arc Czochralski method. A part of the FeSi samples, which were grown with slightly different stoichiometry close to 1:1 were annealed at 1000°C for 3 months. The susceptibility measurements reveal a reduction of the Curie-constant due to the annealing process. In addition, samples with iron excess show a smaller residual susceptibility compared to crystals with iron deficit. This fact cannot be explained by the often claimed assumption that uncompensated iron carries the magnetic moment. The observed appearance of variable range hopping conductivity in combination with a negative magnetoresistivity suggests that Anderson-localized electrons caused by structural disorder induce the low temperature Curie-Weiss-like behavior.

MM 26.8 Tue 14:45 Poster C

First-principles study of the structural and electronic properties of CuO as grown on SrTiO$_3$ — Cesare Franchini[1], Xing-Qiu Chen[2], and •Raimund Podloucky[3] — [1]Faculty of Physics, Univ. of Vienna, Vienna, Austria — [2]Shenyang National Laboratory for Materials Science, Shenyang, China — [3]Faculty of Chemistry, Univ. of Vienna, Vienna, Austria

Very recently, a tetragonal phase of antiferromagnetic CuO was synthesized by growing it epitaxially on a SrTiO$_3$ substrate. In a previous paper [1] we modeled the tetragonal CuO phase by a freestanding block of material simulating the epitaxial effect by fixing the lateral lattice parameters and relaxing the c/a ratio. Applying a hybrid-functional density-functional-theory approach two tetragonal phases were identified whereby the phase with $c/a = 1.38$ perfectly matches the basic experimental structural parameters. However, its electronic structure shows some significant deviations from the experimental valence band spectra. In the present study the effect of the substrate is explicitely taken into account by placing CuO layers with different thicknesses on top of a SrTiO$_3$(100) substrate. Several substrate terminations as well as structural relaxations are considered in order to search for the most stable atomic arrangement. The resulting ground state electronic and structural properties as a function of the thickness of the CuO layer are discussed. For the actual calculations the Vienna Ab initio Simulation Package (VASP) in combination with its hybrid functional features is applied.

[1] X.-Q. Chen et al., Phys. Rev. B **80**, 094527 (2009).

MM 26.9 Tue 14:45 Poster C

Stable and unique solutions for the OEP equation in the LCAO formalism — •julio juan fernandez[1], Christian Kollmar[2], and Michael Filatov[1] — [1]Institute for Advanced Materials, Groningen 9747 AG The Netherlands — [2]Institut fur Physicalische und Theoretische Chemie, Bonn D53115 Germany

The treatment of orbital dependent functionals in Density Functional Theory (DFT) requires the use of the Optimized Effective Potential (OEP) technique for obtaining the local multiplicative potential. Using the exchange only (xOEP) functional this formalism leads to an equation that, in real space, possesses a unique and well defined solution for atoms and molecules. In a basis set (LCAO) scheme the method leads to a non unique solution of the equation due to the singularity of the matrix representation of the linear response operator. In this work we demonstrate that a good solution to this problem is to use an incomplete Cholesky decomposition of the linear response matrix. With the use of this technique numerically stable and unique solutions of the xOEP equations in the LCAO representation are obtained provided that the orbital basis set satisfies the condition of linear dependence of the products of occupied and virtual Kohn_sham orbitals. It is demonstrated that the obtained LCAO-xOEP solutions are independent on the criterion used to discriminate linearly dependent from linearly independent (ia) products.

The LCAO-xOEP solutions for atoms and molecules are obtained with the use of standard basis sets. The LCAO-xOEP energies are in excellent agreement with the numeric real space xOEP energies.

MM 26.10 Tue 14:45 Poster C

Thermomechanical properties of mullite up to 1673 K: single crystal vs. ceramics — •Thomas Friedrich Krenzel[1], Jürgen Schreuer[1], and Hartmut Schneider[2] — [1]Ruhr University Bochum, Institute of Geology, Mineralogy and Geophysics, Bochum, Germany — [2]University of Cologne, Institute of Crystallography, Köln, Germany

The poster by Adel Benlagra originally scheduled for MM 26.10 has been moved to TT 27.21.

Ceramics with mullite composition are well known and appreciated for their favourable properties like high thermal stability, low thermal expansion and conductivity or high creep resistance. They are extensively used as high temperature application materials e.g. like kiln furnitures, catalytic convertors, coatings or engineering ceramics.

Schreuer et al. [1] recently studied the mechanical properties of single crystals up to 1673 K and found an anomaly in the temperature evolution of the strains parallel to principle axes and furthermore a strong deviation from linearity of observed shear stiffnesses compared to calculated ones, both above about 1273 K. They proposed a glass-like transition at this temperature. Another research group interpreted similar or stepwise anomalies of different properties at same temperatures as a phase transition [2; 3].

Since this anomaly is not yet fully clarified the goal of this work is to bring up new aspects by a comparison of thermal expansion and elastic properties of mullite ceramics, which were prepared in different ways, with new single crystal data of higher resolution up to 1673 K. The measurements of thermal expansion and elastic properties were done with the help of dilatometry and resonant ultrasound spectroscopy, respectively.

MM 26.11 Tue 14:45 Poster C

Bestimmung von Fermi-Flächen in dünnen Schichten mittels 2D-ACAR — •Hubert Ceeh, Christoph Hugenschmidt und Peter Böni — Pysik Departement E21, Technische Universität München

Wird ein Positron in einen Festkörper implantiert, thermaliert es innerhalb weniger Picosekunden. Daher ist der Schwerpunktsimpuls des Systems aus Elektron und Positron bei der Annihilation praktisch ausschließlich durch den Impuls des Elektrons bestimmt. Die transversale Impulskomponente führt dabei zu einem von 180 Grad abweichenden Winkel zwischen den Annihilationsquanten. Aus der Messung dieser Winkelkorrelation (ACAR: Angular Correlation of Annihilation Radiation) mittels zweier Anger-Kameras können somit Rückschlüsse auf die Impulsverteilung de Elektronen gezogen werden. Im Gegensatz zu Messungen der Fermifläche unter Ausnutzung des De-Haas-van-Alphen-Effekts sind Messungen mit der ACAR-Methode bei Temperaturen von bis zu 400K möglich. Des Weiteren ist man nicht auf ein starkes Magnetfeld angewiesen, was das Studium der elektronischen Struktur beispielsweise von Supraleitern erlaubt. An der hochintensiven Positronenquelle NEPOMUC wird derzeit ein ACAR-Spektrometer realisiert, um mit mono-energetischen Positronen bei erheblich verkürzter Messzeit, temperaturabhängig die elektronische Struktur in dünnen Schichten untersuchen zu können.

MM 26.12 Tue 14:45 Poster C

Relaxation of Volume and Enthalpy of Bulk Metallic Glasses — •Jonas Bünz, Joachim Bokeloh, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Although the relaxation of glasses is a phenomenon that is known for centuries and that is actually at the very foundations of the unique applicability of glasses in general - the controlled modification of properties without changes of the chemical composition - the physics behind the relaxation and aging processes that occur in glasses after initial quenching are far from being understood. In fact, it is basically still unclear whether the relaxation of the excess free volume and the relaxation of the excess enthalpy are identical processes that are governed by only one underlying mechanism. Measuring the kinetics of these properties with different methods like differential scanning calorimetry, microcalorimetry, dilatometry and the buoyancy method allow covering a broad range of temperatures and materials and offer the possibility to experimentally access the isothermal relaxation characteristics of the volume and the enthalpy directly on time scales that range from several hours to weeks. The results were evaluated in the framework of the free volume theory.

MM 26.13 Tue 14:45 Poster C

The influence of d- and f-states on structure formation - amorphous alloys containing Rare Earths as model systems — •Martin Stiehler, Michael Pleul, and Peter Häussler — Chemnitz University of Technology, 09126 Chemnitz, Germany

Amorphous phases as precursors of the crystalline state are interesting for investigating fundamental structure forming processes and the related evolution of electronic transport. During the last years we were able to show that many different classes of alloys organize themselves under the influence of a resonance interaction between the global subsystems of the electrons and the static structure. Especially for binary Al-TM alloys (TM: the transition metals of the 4th period Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu) we reported recently on an electronic influence on phase stability driven by hybridization effects between the Al-p- and the TM-d-states, showing an interesting systematics depending on the number of unoccupied TM-d-states reflected in different properties. Currently we are about to extend the investigations to systems with transition metals of the 5th and 6th period. Embedded in this class of elements are the so-called Rare Earth metals (Sc, Y, La, and the Lanthanoids). These elements exhibit very similar chemical properties although some of them (the Lanthanoids) contain f-electrons. This provides the possibility of studying the influence of magnetic influences, provided by the localized f-states, on structure formation. In this contribution we report on preliminary results concerning the static structure, the electrical resistivity and the Hall effect of the binary systems Al-Y and Al-Ce.

MM 26.14 Tue 14:45 Poster C

Molecular dynamics simulation of Ni/NiAl interfaces — •Stephen Hocker[1], Siegfried Schmauder[1], and Priyank Kumar[2] — [1]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre, Universität Stuttgart, Stuttgart — [2]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

Molecular dynamics simulations are used to study the brittle/ductile interface Ni/B2-NiAl under mechanical loading. Uniaxial tensile tests perpendicular to the interface are performed. It is shown that interfaces have influence on strain induced material failure by nucleation of defects. Crack propagation in the (001) interface is investigated by applying load via fixed displacement boundary conditions. Determined crack velocities in the interface turned out to be clearly above the crack velocities in each of the respective materials.

MM 26.15 Tue 14:45 Poster C

First-principles study of superhard SiN_x/TiN nanocomposites — •Pawel Rodziewicz and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien ICMM and Computer-Chemie-Centrum CCC, Universität Erlangen–Nürnberg

Nanocomposite materials based on TiN nanocrystalites embedded in an amorphous silicon nitride matrix with thickness of only a few atomic layers and composition close to Si_3N_4 show a superhardness similar to that of diamond. To elucidate the chemical origin of the material hardness and the exceptional strength of the SiN_x/TiN interfaces we have used DFT calculations in combination with Car-Parrinello molecular dynamics (CPMD) simulations to create and to investigate model SiN_x/TiN interface structures. As the first step we studied the initial stages of SiN_x layer formation on TiN(001) by adding successively silicon and nitrogen atoms to the TiN surface to form up to two monolayer thick SiN_x films with different composition. For a selected set of configurations, chosen on the basis of thermodynamic stability, we then applied a stepwise procedure based on heating, quenching and final geometry optimization to search for stable and energetically favorable amorphous structures of SiN_x films and stacks of SiN_x/TiN multilayers. The relative stability of the different model interface structures is analyzed in terms of Ti, Si and N coordination numbers, and the mechanical strength of the interfaces is assessed by the calculation of stress–strain curves to determine the ideal decohesion strength.

MM 26.16 Tue 14:45 Poster C

Tailoring Model Surfaces and Wettability Measurement for a Fundamental Understanding of Hot-dip Galvanizing — •Takashi Kawano[1,2] and Frank U Renner[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Steel Research Laboratory, JFE Steel Corporation, Japan

Hot-dip galvanizing is the process used widely for automotive steel sheets. The wettability of molten Zn with steel substrate is an important issue in the process. Especially, problems can be caused by substances such as Al, Si and/or Mn oxides formed on a substrate surface during the process. Many studies have been done to correlate the wettability and sample composition and/or process conditions related to the practical steel materials or process procedure.

However, the affect of the oxides on the wetting kinetics has not been well explained, because the surfaces of such steel substrates are generally too complicated to understand the fundamental wetting mechanisms.

Our work was started with preparing simple model surfaces so that fundamental wetting kinetics on well defined substrates can be studied with the sessile drop method at high temperatures. Our model surfaces were well defined oxide islands prepared by physical vapor deposition using different masks on flat Fe substrates.

In this report, preliminary data which shows a relation between initial contact angle and Al oxide coverage will be introduced. Comparing among various kinds of oxide species and modeling of the wetting kinetics will be future work.

MM 26.17 Tue 14:45 Poster C

Theoretical investigation of the adsorption of SPS and MPS at the Cl-covered Cu(100) surface — •W. Reckien[1], N.T.M. Hai[2], A. Fluegel[3], W. M. Hahn[3], A. Wagner[3], D. Mayer[3], P. Broekmann[2,3], and T. Bredow[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Department of Chemistry and Biochemistry, University of Bern, Switzerland — [3]BASF-SE, Electronic Materials, Ludwigshafen, Germany

Copper electrodeposition has attracted considerable attention over the last two decades due to its application in the state-of-the-art fabrication of integrated logic and memory devices. A detailed understanding of the synergistic and antagonistic interaction between so-called accelerator, suppressor and leveller molecules among themselfes and with the chlorine covered copper surface is still lacking.

We present the results of a first principles study of the interaction of the accelerator molecule SPS (bis-sodiumsulfopropyl-disulfide) and the corresponding MPS (mercaptopropylsulfonic acid) monomer with the Cu(100)/Cl system. We discuss different adsorption situations on the pure Cu(100) surface, on a compact c(2 x 2)-Cl adlayer and the influence of chlorine defects in the adlayer. Since the consideration of the electrolyte is crucial for an accurate description of the process, we present new models for the adsorption of SPS and MPS in the presence of a water electrolyte.

MM 26.18 Tue 14:45 Poster C

Ab-initio investigation of the interface structure of TiO_2 grown on Al_2O_3 — •Maxim Popov[1,2], Jürgen Spitaler[1,2], Claudia Walter[2], and Claudia Ambrosch-Draxl[2] — [1]Materials Center Leoben Forschung G.m.b.H, Rosegger-str. 12, 8700 Leoben, Austria — [2]Montanuniversität Leoben, Franz-Josef-Str. 18, 8700 Leoben, Austria

Oxide based layered structures are increasingly exploited for hard coatings. As a model system we study the interface between a TiO_2 thin film grown on an Al_2O_3 (0 0 0 1) substrate by sputter deposition. X-ray diffraction analysis of the sample reveals that TiO_2 grows in the rutile structure with the (1 0 0) plane parallel to the substrate. We use ab-initio calculations based on density-functional theory (DFT) combined with elasticity considerations to determine the local atomic arrangement at the interface region. Since the two materials forming the interface exhibit a rather large lattice mismatch, we first calculate the full elastic constant tensors for bulk Al_2O_3 and TiO_2. Then the interface between Al_2O_3 and TiO_2 is constructed by connecting the two surfaces in such a way that the stresses on both sides are balanced. In a next step the geometry of the complete interface is further relaxed within DFT. We present the optimized interface structure for three interfaces differing in the termination of the substrate or overlayer,respectively.

MM 26.19 Tue 14:45 Poster C

Ordering and site occupancy of ternary elements in Fe_3Al — •Thomas Rademacher[1], Thomas Kresse[1], Johannes Deges[2], Talaat Al-Kassab[3], Georg Frommeyer[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]MPI für Eisenforschung GmbH, Max-Planck-Straße 1,40237 Düsseldorf, Germany — [3]King Abdullah University of Science & Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

$D0_3$-ordered Fe_3Al exhibits a number of advantageous properties, such as high-temperature strength, corrosion resistance and low cost. However, the mechanical properties (e.g. low ductility) and high-temperature stability needs to be optimized for technical use which can be performed by the addition of ternary elements. To understand their influence on these properties, the site occupancy needs to be determined.

In this study this is investigated for the ternary elements 4at.%V, 5at.%Cr, 5at.%Mn and 4at.%Ti 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. By comparing these APT-measurements with APT-simulations for different site occupancies and orderings, measurement artefacts can be extracted and an enhanced analysis can be performed.

MM 26.20 Tue 14:45 Poster C

X-ray diffraction studies on diamond cobalt composites — •Andre Steffen[1], Christian Kronholz[2], Michael Paulus[1], Christoph J. Sahle[1], Manuel Ferreira[2], Wolfgang Tillmann[2], and Metin Tolan[1] — [1]TU Dortmund, Experimentelle Physik 1 / DELTA — [2]TU Dortmund, Lehrstuhl für Werkstofftechnologie

Diamond grinding tools have widely established its usage in machining and cutting of natural stone and concrete. The interface area between diamonds and cobalt in diamond cobalt composites is of essential relevance for the grinding process and has been investigated by X-ray diffraction (XRD) studies. It could be shown that graphite is formed during the manufacturing process and that graphite is the main constituent of the diamond cobalt interface area. No strong (chemical) bonding in the form of cobalt carbide could be detected. By in situ and ex situ studies on ultra fine cobalt powders the thermal induced phase transformation between face centered cubic and hexagonal closed package phase of cobalt at T=421 °C has been investigated. At T=620 °C cobalt occures only in the fcc phase while both phases exist at room temperature (RT). The phase transformation, fcc to hcp during cooling from T>421 °C to RT, strongly depends on the cooling gradient. Furthermore it could be shown that the phase transformation, fcc to hcp, can be additionally induced by pressure. High pressure (P=550 MPa) leads to a high volume fraction of hcp phase (about 95 %).

MM 26.21 Tue 14:45 Poster C

Anisotropic mechanical behavior of the ultrafine grained TiFe eutectic system — Antje Schlieter, •Uta Kühn, and Jürgen Eckert — Helmholtzstrasse 20, IFW Dresden, 01171

The effect of temperature gradient and growth rate of an eutectic TiFe alloy have been examined. Samples have been arc melted ingots, cold crucible and tilt cast rods and rods cast by Bridgeman technique. The material exhibit different nanoscaled/ultrafine grained (ns/ufg) eutectic structure (β-Ti(Fe) solid solution (ss) + TiFe). Different cooling conditions lead to the evolution of ufg eutectic colonies with different orientation versus elongated lamella colonies with preferred orientation. Consequently, isotropic versus anisotropic mechanical properties were obtained. The alloys exhibit compressive strengths between 2200 - 2700 MPa and plasticity in the range of 7 to 19 % in compression.

MM 26.22 Tue 14:45 Poster C

Deformation of Au Nanoparticles — •Andreas Kelling, Burkhard Roos, and Cynthia A. Volkert — Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen

Compression experiments and TEM investigations have been performed on Au nanoparticles with diameters between 80 and 250 nm in an effort to understand nucleation and motion of dislocations in small volumes. TEM images of the 80 nm nanoparticles confirm that they are twinned in their as-received condition, but that the twins can be annealed out by heating to 400°C. Compression of the 250 nm diameter particles with a flat punch in a nanoindenter gives reproducible force-displacement curves, allowing controlled deformation of the nanoparticles to the desired strain. In preparation for TEM investigations of the deformed nanoparticles, compression tests have been performed on 80 nm diameter nanoparticles placed on a TEM-transparent SiN membrane. By investigating the stored dislocations in the deformed nanoparticles, it is hoped that insights will be gained into the mechanisms that lead to the high strength of sub-micrometer metal specimens.

MM 26.23 Tue 14:45 Poster C

SPM Studies of Dislocations in Deformed Au Thin Films — •Sönke Schmidt[1], Alissa Wiengarten[1,2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]now at TU Berlin

The high strength of metal thin films relative to bulk materials is attributed to the inhibition of dislocation activation in small volumes, but the exact mechanisms are not clear. Studying dislocation-controlled deformation of thin films requires high resolution techniques such as TEM or SPM. In contrast to in-situ deformation in the TEM, in-situ SPM investigations do not require special sample preparation and provide quantitative Burgers vector information. However, they have poorer time resolution and can only image dislocations where they intersect the surface. In this study atomically flat gold thin films of about 100 nm thickness and a grain size of about 400 nm, produced by a template method on glass substrates, were investigated both in STM and AFM. Deformation of the films was performed by indentation of the tips into the sample surface. For future studies, these thin films will be transferred to deformable substrates, where they will be used for in-situ tensile test during AFM imaging.

MM 26.24 Tue 14:45 Poster C

In-situ SEM tensile testing of single crystal Au nanowires — •Bahne Kapelle[1], Gunther Richter[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Max-Planck-Institut für Metallforschung, Stuttgart

The deformation behavior of nanoscale metals differs from that of bulk metals, showing in particular an increase in strength with decreasing size. The aim of this study is to determine the deformation process and strength of high quality single crystal Au nanowires using in-situ tensile testing in the SEM. Nanowires with diameters between 75 and 250 nm are mounted in a tensile setup using a micromanipulator and Pt deposition. The force on the wires is measured using a capacitive MEMS device during displacement controlled loading with a piezoelectric actuator. First results on a 180 nm diameter nanowire show homogeneous deformation up to $\approx$10% strain, followed by localized deformation and ductile rupture. Stress-strain curves and deformation morphologies for various diameter wires will be presented and interpreted in terms of in-situ TEM observations of dislocation activity obtained from the same wires in a separate study.

MM 26.25 Tue 14:45 Poster C

Automated dislocation detection in atomistic simulations — •Alexander Stukowski, Jonathan Schäfer, and Karsten Albe — FB Materialwissenschaft, TU Darmstadt, Germany

We present a novel method that allows us to directly extract dislocation lines and their associated Burgers vectors from atomistic simulations. Our dislocation detection algorithm is based on an automated Burgers circuit analysis to trace dislocation cores followed by a vectorization step, thereby achieving the transition from the atomistic system to a discrete dislocation representation.

The dislocation analysis can be efficiently performed on-the-fly during molecular dynamics (MD) simulations with a high time resolution. This enables the investigation of rapid dislocation processes, whose observation was otherwise impeded by other crystal defects or simply by the huge amount of data produced by large-scale MD simulations.

Our analysis method can reliably detect perfect, partial, and twinning dislocations. For the first time, the dislocation density in MD simulations can now directly be quantified. In principle, even more comprehensive data not accessible before can be extracted, including dislocation mobility and dislocation reactions.

The new analysis method is applied to large-scale deformation simulations of nanocrystalline metals to study the density and character of dislocations as a function of strain. Being able to directly visualize and measure dislocation activity gives new insights into the interplay of grain-boundary mediated processes and dislocation plasticity in such materials.

MM 26.26 Tue 14:45 Poster C

Thickness Effects in Very High Cycle Fatigue Behavior of Cu Films — •Clemens Trinks, Felix Hebenstreit, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

It has recently been established that decreasing the thickness of metal films leads to an increase in fatigue life and a change in fatigue damage morphology. This has been correlated with the high strength of thin films and attributed to their limited dislocation activity. The current research extends fatigue studies below 100 nm film thickness and to ultra high cycle numbers. Such studies are of great relevance for predicting the reliability of metal components used in micro- and nanotechnology, where they often experience repeated, low-level mechanical or thermal-mechanical loading. A resonant cantilever method has been developed using an AFM to test and monitor the fatigue behavior of

Cu films with thicknesses between 20 nm and 2 μm. Strain amplitudes up to 0.1 % and cycle numbers up to 10^{10} have been achieved. First results from a 200 nm thick film show evidence of narrow extrusions parallel and next to twin boundaries, as well as cracking and grooving at grain boundaries. This damage is similar to what is observed in low cycle fatigued films of similar thickness, giving first indications that the mechanisms of damage formation are determined predominately by the film thickness and not by the strain amplitude.

MM 26.27 Tue 14:45 Poster C

Strukturelle Umwandlungen von Niederdruckpolyäthylen bei mechanischer Beanspruchung — •Heinz Hans Walter Preuss — Hameln

Es werden die bislang weitgehend unbeachtet gebliebenen Ergebnisse der elektronenmikroskopischen Untersuchung [1] struktureller Umwandlungen von Proben aus Niederdruckpolyäthylen bei mechanischer Beanspruchung vorgestellt. Gezeigt wird, dass die mit dem Faltungsmodell nach Keller [2, 3, 4] gedeuteten Lamellen sich mechanisch voneinander trennen lassen, indem galvanisch mit Kupfer verstärkte Aufdampfschichten aus Gold von der Oberfläche sphärolithisch aus der Schmelze erstarrter Polyäthylenproben abgezogen werden. Mit direkten elektronenmikroskopischen Durchstrahlungsuntersuchungen lässt sich zeigen, dass die sphärolithische Struktur dünner Polyäthylenhäutchen sich beim Zerreißen übergangslos in Faserstrukturen umwandelt. Beim makrospröden Bruch massiver Polyäthylenproben bei Raumtemperatur und bei *195oC lässt sich sowohl die Umwandlung in Faserstrukturen als auch dass Erreichen der Schmelztemperatur bruchflächenmorphologisch nachweisen. Literatur: 1 A. Keller, Phil. Mag. /8/ 2, (1957), 1171 2 H. H. W. Preuß, Dissertation, Leipzig 1963 3 H. H. W. Preuß, physica status solidi, 3 (1963), Nr. 3, K109 ff. 4 H. H. W. Preuß, Plaste und Kautschuk, 10 (1963) Nr. 6, 330 ff.

MM 26.28 Tue 14:45 Poster C

Elastic: A program for calculating elastic constants for arbitrary lattice types based on ab-initio total energies — •Rostam Golesorkhtabar[1,2], Jürgen Spitaler[1,2], Peter Puschnig[2], and Claudia Ambrosch-Draxl[2] — [1]Materials Center Leoben Forschung G.m.b.H, Rosegger-str. 12, 8700 Leoben, Austria — [2]Montanuniversität Leoben, Franz-Josef-str. 18, 8700 Leoben, Austria

Detailed informations about elastic properties play a key role in material science and technology. On an atomistic level, this information is represented by the elastic tensor. We have present Elastic, a code that is able to calculate the full elastic tensor for any crystal structure from ab-initio total energies. For this purpose, structure files with special distortions corresponding to the lattice type are created. Then the total energies of all structures are determined from ab-initio calculations within density-functional theory, which are then fitted to the applied strains in order to get all independent elements of the elastic tensor. Based on the elastic tensor our program calculates the elastic compliances, the bulk, shear and Young moduli and the Poisson ratio. By using both, the Voigt and the Reuss averaging, the ab-initio results are related the elastic properties of polycrystalline samples. From symmetry considerations all space groups can be classified into 9 types differing in the number of independent components of the elastic tensor. We have tested our program for one representative of each class, using total energies obtained with the full-potential linearized augmented plane wave code WIEN2k, and compare the results with experimental data from literature.

MM 26.29 Tue 14:45 Poster C

Nanoantennae from high melting point transition metal nanowires — •Litty Varghese Thekkekara[1], Andreas Erbe[1], Diedrich A Schmidt[2], Martina Havenith[2], and Achim W Hassel[1] — [1]Max-Planck Institute für Eisenforschung,Düsseldorf — [2]Lehrstuhl für Physikalische Chemie II, Ruhr University, Bochum

Due to their optical properties, nano metallic objects attract considerable attention in various fields of nanotechnology, such as thermal emitters, sensor applications, and analytical bioscience.

Here, nanowires were prepared by electrochemical etching from directionally solidified eutectic alloys (NiAlX, X =Mo, Re, W) and transferred to infrared-transparent substrates, mainly silicon.We have performed optical and morphological characterization of single, high melting point transition metal nanowires (rhenium, molybdenum and tungsten) with high aspect ratios and a thin protective oxide layer. Nanowire morphologies were confirmed using scanning electron microscopy as well as atomic force microscopy. The length of the wires is ˜100μm,at a width of ˜400nm.

Optical properties were measured using infrared micro spectroscopy. Small metal nanostructures with high aspect ratio do normally show a strong antenna-like longitudinal plasmon mode at a wavelength λ ˜ 2L (L- length). Due to the length of the wires studied here, this mode is expected to be excited in the far infrared wavelength range.

MM 26.30 Tue 14:45 Poster C

Electronic Properties of Graphene Nanoribbons — •Ezgi Erdogan and Gotthard Seifert — Theoretische Chemie, TU Dresden, 01062 Dresden

The aim of present work is to review the electronic properties of Graphene nanoribbons (GNR) with the density functional tight binding method (DFTB) based on molecular dynamics (MD) simulation in the NVT ensemble for investigating energy gaps, defect area, strain effect and to understand switching between metallic and semiconducting properties. MD simulations are performed on Armchair GNR (AGNR) with (12,7,196) and (17,7,266) indexes and Zigzag GNR (ZGNR) with (20,9,198) and (22,9,216) indexes. The indexes (a,b,c) refer to 'a' - the width in number of carbon atoms, 'b' - the unit cell and 'c' - the total number of atoms in the configuration of the graphene sheet. The Graphene edges are saturated by hydrogen atoms. AGNRs are always semiconducting. The AGNR(12) has a 0.7 eV gap. During stretching process, one or two C-atom chains remain between two graphene halves. DOS pretends a switch to metallicity at a strain of 16%, but for the chain of single carbon atoms a band gap is visible in local density of states (LDOS). For AGNRs no change from semiconducting to metallic behavior for any value of strain is observed in transport calculations with a Green's function method. In contrast, ZGNRs remain conducting.

MM 26.31 Tue 14:45 Poster C

Aggregation of carbon in a H_2 atmosphere investigated by ReaxFF-molecular dynamics simulations — •Norbert Lümmen — University of Bergen, Department of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Controlled manufacturing of very pure carbon nanoparticles (Carbon Black) can be achieved by, for example, thermal decomposition of gaseous precursors like acetylene or methane. A large quantity of molecular hydrogen is produced during the decomposition process.

We have investigated the aggregation process of carbon molecules and hydrocarbons from carbon atoms in an atmosphere of H_2 at different temperatures, densities and initial amount of H_2 by molecular dynamics (MD) simulations. The calculation of interatomic forces within the MD-simulations was based on the Reax Force Field (ReaxFF).[1]

The growth of molecules and their compositional changes were followed up to 4 ns of simulation time. The developing number of ring structures based on carbon atoms was analysed by the shortest-path ring method.[2] Formation of carbon catenates and hydrocarbons of different sizes was observed. A decreasing amount of initial H_2 allows the aggregation of pure carbon molecules up to 30 atoms. Hydrogen atoms are found along and at the ends of these carbon chains in all types of systems. These linear molecules eventually aggregate to larger ones in which networks of rings of carbon atoms can be found.

[1] van Duin et al., J. Phys. Chem. A 105, 9396 (2001).
[2] Franzblau, Phys. Rev. B 44, 4925 (1991).

MM 26.32 Tue 14:45 Poster C

Mechanical Characterization of Layered Nanocomposites — •Inga Knorr, Susanne Seyffarth, Tobias Liese, Hans-Ulrich Krebs, and Cynthia A. Volkert — Institut für Materialphysik, Universität Göttingen

Multilayer thin films with dimensions at the nanometer scale represent a technologically important class of materials which can offer improved mechanical properties as a result of composite and size effects. The samples studied here consist of Cu/PMMA- and Ti/ZrO_2-multilayer films produced using pulsed laser deposition. Mechanical characterization is performed in a nanoindenter using Berkovich indentation as well as micro-compression tests on columns machined from the films with a focused ion beam microscope. Furthermore, the morphology of the samples in the undeformed and deformed states is investigated with SEM and TEM. The goal of the studies presented here is to gain information about the size-dependence of the layer mechanical properties as well as to identify deformation and failure mechanisms in multilayered samples. Details about the mechanical properties of films with layer thicknesses between 5 and 1000nm will be presented. The dependence of mechanical behavior and deformation morphology on layer dimensions will be discussed.

MM 26.33 Tue 14:45 Poster C

Structural and electrochemical properties of mixed transition metal phospho-olivine systems — •Michaela Memm, Peter Axmann, and Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Helmholtzstraße 8 89081 Ulm

lithium iron phosphate LiFePO4 shows a very good cycling stability at a potential of 3.5 V vs. Li/Li+ with a specific capacity of up to 160 mAh/g at room temperature. the potential and other properties of the phospho-olivines can be influenced by substituting other transition metals, such as manganese, cobalt and nickel, for iron. the transition metal phospho olivines can form solid solutions, among which LiFexMn1-xPO4 is a well known system. In this work, we prepared and characterized binary and ternary series of phospho olivines with M = Co, Mn, Fe, Mg. the systems form solid solution series LiCo1-xMxPO4 for M = Fe, Co and LiMgxFeyMn1-x-yPO4. The particle morphology is strongly influenced by M. A two step potential characteristic is observed for the mixed systems LiCo1-xMxPO4 and LiMgxFeyMn1-x-yPO4 with the single steps occurring on potential close to those of the pure end members. Significant potential shifts can be observed depending on the composition. We found high capacity yields for the Mg containing samples

MM 26.34 Tue 14:45 Poster C

Resistance measurements on a single nanoparticle and nanoparticle ensembles — •Ivan S. Titov, Marina Spasova, and Michael Farle — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany

In this work the resistance of 18 nm iron oxide nanocubes was measured using Scanning Tunneling Microscope mounted inside of Transmission Electron Microscope (TEM-STM technique). Chain-like structures consisting of the arbitrary numbers of the cubes were built using tungsten STM tips. The process of the chain formation was visualized in TEM. Voltage-current curves for a single nanocube and nanocube chains were recorded in a contact STM mode using gold and tungsten tips. Correlation of electrical properties with the structure and the chain morphology as well as influence of contact resistance and deformation of the samples on measured resistance values are discussed. The work is supported by DFG/SFB 445.

MM 26.35 Tue 14:45 Poster C

Near Surface Lattice Relaxation in Transition Metal Nanoparticles — •Björn Bieniek, Darius Pohl, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany

The near-surface lattice relaxation of transition metal alloy nanoparticles is investigated. Recent results show that CuAu and FePt particles show a pronounced lattice expansion of about 10% at their surface. Here, MD simulations indicate that the segregation of the heavier elements (Au, Pt) leads to the experimentally observed lattice expansion. However, surface-sensitive XAS and PES have revealed the presence of oxygen in the surface layers of FePt particles which could in turn contribute to and/or cause the expansion of the lattice. To investigate the influence of oxygen on the near-surface lattice expansion, FeNi particles are investigated. FeNi is much more susceptible to oxidation than CuAu and FePt. In contrast to the latter, abberation-corrected high resolution TEM on FeNi particles reveals that metallic particle cores are surrounded by crystalline oxide shells. Almost no lattice relaxation is observed in the metallic core, and the interface between the metal and the oxide is atomically sharp. Both, defects due to the lattice mismatch at the interface and a significant lattice relaxation are *only* observed in the oxide shell. MD Simulations and HRTEM contrast simulations of FeNi nanoparticles are presented to confirm the experimental results.

MM 26.36 Tue 14:45 Poster C

Adjusting the Size of Nanochannels in Silicon and Silicon Oxide Samples — •René Berwanger and Rolf Pelster — FR 7.2 - Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have prepared free-standing porous silicon layers by electrochemical etching of heavily p-doped silicon wafers. Pore size and porosity are analysed via nitrogen isotherms. With increasing etching time the thickness of the samples, the average pore radius and the porosity increase (r = 3 nm - 7 nm). Completely oxidized and transparent samples are obtained by heat treatment. This procedure does not affect the average pore radius although the total sample volume increases. Such a decrease of porosity can be explained with a simple model. These samples where used for measurements on confined n-alcohols. For some short-chain alcohols, which crystallize under normal condition, the confinement induces a glass transition.

MM 26.37 Tue 14:45 Poster C

Nanocrystalline $LiFePO_4$ Prepared by Mechanochemical Route — •Vladimir Šepelák[1], Sylvio Indris[1], Klaus Dieter Becker[2], Wolfgang Bensch[3], and Paul Heitjans[4] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Braunschweig University of Technology, Braunschweig, Germany — [3]Christian-Albrechts-University Kiel, Kiel, Germany — [4]Leibniz University Hannover, Hannover, Germany

Among the typical Li ion battery cathode materials, $LiFePO_4$ of the phospho-olivine family is particularly interesting due to its high power density, low cost, and environmental compatibility. Taking into account a nonequilibrium state of complex oxides prepared by mechanochemical methods [1], an enhanced electrochemical performance may be anticipated in such 'interface-controlled' materials.

In the present work, nanocrystalline $LiFePO_4$ with an average particle size of about 10 nm was prepared via far-from-equilibrium mechanochemical processing of the bulk $LiFePO_4$. HR-TEM studies revealed a nonuniform structure of $LiFePO_4$ nanoparticles consisting of an ordered core surrounded by a disordered surface shell/interface region. A comparative ^{57}Fe Mössbauer spectroscopic study of bulk and nanocrystalline $LiFePO_4$ revealed that the near-surface layers of phosphate nanoparticles are disordered due to the strongly distorted geometry of the FeO_6 octahedra. Quantitative information on hyperfine parameters of the nonequilibrium $LiFePO_4$ nanophase is obtained.

The work is supported by the DFG (SPP 1415).

[1] V. Šepelák et al., Chem. Mater. 21 (2009) 2518.

MM 26.38 Tue 14:45 Poster C

Finite-Size effects in GaN nanoparticles studied by a novel dynamic-charge transfer potential — •Manuel Diehm, Peter Agoston, and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt

Nanoparticles of compound semiconductors exhibit a number of peculiar properties, including phase transitions and unusual structural relaxations. Atomic scale modelling of such effects by quantum mechanical ab-initio calculations is, however, computationally too demanding, while classical potentials are limited to fixed charge models or computationally costly charge equilibration schemes. In this contribution, a novel dynamic charge-transfer bond-order potential (DCT-BOP) is applied, which opens the possibility to study larger ionic systems with variable charge states. The variability of the charges may carry great importance when modelling nanoparticles, since a reduction in the charge state of an ion can mitigate the impact of missing Coulomb interactions at surfaces or defects and change the energetics of relaxation. Here, we present calculations on Gallium Nitride nanoparticles using the DCT-BOP in comparison to a conventional bond-order potential and a pure Coulomb/Buckingham Potential. We examine the size dependence of charge states, relaxation energy gain and the interplay of surface and bulk contributions.

MM 26.39 Tue 14:45 Poster C

Low Energy Excitations in Semiconductor Nanoparticles — •Andreas Hartmann[1], Darius Pohl[1], Ludwig Schultz[1], Stephen Hickey[2], Alexander Eychmüller[2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, Physical Chemistry and Electrochemistry, Bergstr. 66b, D-01062 Dresden, Germany

Low energy excitations such as plasmons or excitons and also the semiconductor band gap usually depend strongly on the dimensionality and the size of the material. As a consequence, the control of various electronic properties of semiconductor nanoparticles by merely controlling their size is since long a vital research field. The vast majority of the investigations is, however, focussed on characterising the properties of particle ensembles, and only little work is so far dedicated to the correlation of size, structure, and electronic properties in individual isolated particles. Modern aberration-corrected HRTEM in combination with local EELS provides an effective tool to investigate such correlations. The potential of using HRTEM with a monochromated electron source at low acceleration voltages offers new opertunities to characterize low energy excitations with high energy and spatial resolutions. Here, the effective suppression of Cerenkov radiation backgrounds upon reducing the acceleration voltage and the gain in energy resolution by using a monochromated beam is largely beneficial to low energy EELS. The potential and the limitations of this method are explored for the example of colloidal wide band gap Zn-O nanoparticles.

MM 26.40 Tue 14:45 Poster C

Phase-field simulation using the Calphad method — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Materials and Processes, Karlsruhe, Germany

The strength of the phase-field method to simulate material alloy systems has been demonstrated over the years. This requires the knowledge of the Gibbs-free energy of the phases involved in the transition. The Calphad method involves the calculation of phase diagrams of multi-component systems, using datasets generated through comparative studies with experiments and density functional theory calculations. This methodology has gained popularity for use in simulations and experimental studies, as this includes a creditable collection of the Gibbs-free energies of a number of material systems. Databases are available for most binary systems, and a number of ternary systems of technical interest. In the present study, we build the methodology for the direct use of the databases in the simulation of material alloys, using the phase-field method. In particular, we investigate the Al-Si system, given the wide range of microstructures possible and its significance in the industry.

MM 26.41 Tue 14:45 Poster C

Crystallization and Phase Separation of $Si_{1-x}C_x$ (x = 0.33) Films — •Kai Volgmann[1], Wolfgang Gruber[2], Harald Schmidt[2,3], Wolfgang Maus-Friedrichs[1,3], Udo Geckle[4], and Michael Bruns[4] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, D-38678 Clausthal-Zellerfeld — [2]Institut für Metallurgie, AG Materialphysik, TU Clausthal, D-38678 Clausthal-Zellerfeld — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, D-38678 Clausthal-Zellerfeld — [4]Institut für Materialforschung III, Forschungszentrum Karlsruhe GmbH, D-76344 Eggenstein-Leopoldshafen

Microstuctural changes during annealing of amorphous silicon carbide with varying silicon to carbon ratios are of considerable interest for tailoring of material properties in view of technical applications. We investigated phase separation and crystallization behaviour of magnetron sputtered amorphous $Si_{1-x}C_x$ films (x = 0.33) with a thickness of 1.4 μm deposited on Si substrates using XPS, GI-XRD and SIMS. For as deposited samples XPS confirm a Si/C ratio of 2:1. After annealing at 700 °C for 30 min the samples are still amorphous but XPS reveal a Si/C ratio of 1.33. The information depth of XPS is about 10 nm. During isothermal annealing at higher temperatures between 1200 and 1350 °C GI-XRD shows first the simultaneous formation of crystalline Si and nanocrystalline SiC. Further annealing leads to a continuous decrease and complete vanishing of crystalline Si, while the amount of SiC increases until fully crystallization. The temperature dependence and possible explanations of this effect are discussed.

MM 26.42 Tue 14:45 Poster C

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

Phase-change materials are one of the most promising candidates for future memory technology applications and are presently considered to replace FLASH-Memory or even DRAM. The non-volatility of the stored data is a key feature of these phase-change memories, which is enabled by a permanent structural rearrangement: the switching between a highly resistive amorphous state and a low resistance crystalline one. The fundamental mechanism of crystallization in these materials is still not fully understood. That's why a comprehensive investigation of the temperature dependence of crystal nucleation and growth is highly desirable. However, within the temperature regime between the glass transition temperature and the melting point, phase-change materials possess an extremely fast crystallization speed. Therefore a new optical in-situ tester has been assembled to tackle this challenge 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. The measurement principle is demonstrated using AgInSbTe, a typical phase change material known from optical data storage.

MM 26.43 Tue 14:45 Poster C

Simulations of the martensitic phase transition in NiTi — •Daniel Mutter and Peter Nielaba — Physics Department, University of Konstanz, 78457 Konstanz, Germany

In this work, molecular dynamics simulations of the martensitic phase transformation of NiTi are performed, which occurs between the low-temperature B19' structure and the high temperature B2 structure. This effect is the reason for the shape memory behaviour and the extraordinary superelasticity of NiTi, which make it one of the most commonly used shape memory alloys in engineering.

In order to explore the possibility to use these effects at the nanoscale, the simulations were carried out in a range of about 1000 - 4000 particles, with a potential arising from the tight binding model in the second moment approximation ([1]).

By analyzing the deformation of the simulation box and the crystal structure during a heating-cooling process, it is shown, that the B19' structure is stable at low temperatures and that the phase transition occurs at about 310 K for equiatomic NiTi. Further results show an extreme concentration dependence of the martensitic transition temperature, as well as the behaviour of the Gibbs free energy during the phase changes.

Because of a few not well reproduced experimental facts, first simulations with an improved potential ("modified embedded atom method" [2]) are presented.

[1] W. S. Lai, B. X. Liu, J. Phys. Cond. Mat. **12**, L53-L60 (2000).

[2] Y.-M. Kim *et al.*, Phys. Rev. B **74**, 014101 (2006).

MM 26.44 Tue 14:45 Poster C

Molecular Dynamics Simulations of Laser Ablation in orthorhombic $Al_{13}Co_4$ — •Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

Femtosecond laser ablation of the Aluminum-Cobalt alloy $Al_{13}Co_4$ is investigated. For the simulations of the lattice ions we use molecular dynamics, while for the time evolution of the electron-temperature a generalized heat-conduction equation is solved by a finite difference scheme. Energy transfer between the subsystems is allowed by 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]. The alloy shows large structural affinity to decagonal quasicrystals, which have an *in-plane* five-fold symmetry, while in perpendicular direction the planes are stacked periodically. As a consequence we observe slight anisotropic melting behavior.

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

MM 26.45 Tue 14:45 Poster C

Seed induced nucleation in colloidal model systems under microgravity — •Patrick Wette[1] and Hans Joachim Schöpe[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz

Understanding the process that drives an under cooled fluid to the crystal state is still a challenging issue for condensed matter physics and plays a key role designing new materials. Crystallization undergoes crystal nucleation, growth and ripening. The crystallization kinetics and the resulting polycrystalline morphology are given by a complex interplay of these mechanisms. A great deal of progress has been made in recent years using colloidal suspensions as model system studying crystallization. We here present systematic measurements of the crystallization kinetics of a charged colloidal model system adding small amounts of seeds using time resolved scattering techniques. Large seeds show strong sedimentation under gravity even on the timescale of the crystallization process. To avoid this problem we performed our measurements under micro gravity during parabolic flights. We report how the seeds size and structure affect crystal nucleation and growth as function of meta stability giving the possibility to modify the crystallization process.

MM 26.46 Tue 14:45 Poster C

Phase transitions of colloidal monolayers on decagonal light induced substrates — Günther Gera, •Thomas Bohlein, Jules Mikhael, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Two dimensional phase transitions remain of high interest to a broad scientific community. According to KTHNY theory, melting in 2D occurs via two sequential defect-driven phase transitions. In this context colloidal systems, having a multitude of accessible interactions, offer a suitable way to investigate such phenomena in real space. Most of the work considered 2D colloidal systems with only mutual interactions, or in few cases interaction with underlying periodic substrate potentials. Here we report measurements of the complex phase behavior of a triangular colloidal monolayer in the presence of a quasiperiodic substrate potential acting via optical forces on the particles. Experimentally, it is created by interfering 5 laser beams. This potential, although not periodic, has a long range order and a decagonal rotational symmetry. At different potential strengths several phenomena are depicted. At low laser intensities, reorientation of the high symmetry axis of the crystal is observed. For higher intensities, we identify the typical geometrical point defects which mediate the transition to the quasicrystalline phase. Here, the structure factor exhibits the decagonal symmetry as expected. For certain densities, line defects lead to a transition to the Archimedean-like tiling phase.

MM 26.47 Tue 14:45 Poster C

Studies on phason flips by kinetic Monte Carlo simulations — •Hansjörg Lipp and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Stuttgart

Neutron scattering experiments [1] indicate that atoms in quasicrystals perform flips between split positions with typical time scales of picoseconds. On the other hand, Edagawa et al. have presented HRTEM images [2], where bright spots are flipping with periods of seconds or even minutes.

To explain this apparent discrepancy, we start from a structure model for d-Al-Cu-Co of Zeger et al. [3], where a ring of ten atoms can perform a jump by four consecutive single atom flips. By applying kinetic Monte Carlo simulations [4], we study how these collective flips, which occur in the different layers of the d-phase can lead to flips detectable by HRTEM on much lower frequency scales.

[1] G. Coddens *et al.*, *Phys. Rev. Lett.* **78**, 4209 (1997)
[2] K. Edagawa *et al.*, *Phys. Rev. Lett.* **85**, 1674 (2000)
[3] G. Zeger and H.-R. Trebin, *Phys. Rev. B* **54**, R720 (1996)
[4] A. B. Bortz *et al.*, *J. Comput. Phys.* **17**, 10 (1975)

MM 26.48 Tue 14:45 Poster C

Vapour galvanizing (Sherardizing) of Copper with Zinc — •Dietbert Wortelen[1], Hartmut Bracht[1], Frank Natrup[2], and Wolfram Graf[2] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]Bodycote Wärmebehandlung GmbH, Sprockhövel, Germany

Using a vapour galvanizing technique called Sherardizing we investigated the growth kinetics and coefficients of zinc copper phases. For this purpose polished (OFHC)-copper plates and zinc powder have been sealed in quartz ampoules under inert gas atmospheres and annealed at a temperature range between 300 and 410°C. In order to study the coating thickness and the phase composition, cross sections were prepared, which have been analyzed by means of optical microscopy and scanning electron microscopy. We were able to demonstrate that the coating thickness is a function of the parabolic time law and that the formed coatings are composed of two layers referring to the ordered beta-CuZn and gamma-Cu5Zn8-phases. To enhance the coating quality, small amounts of ZnCl2 were added to the zinc powder. It was observed that the coating thickness decreased with increasing ZnCl2. Experiments with variable Ar-pressure demonstrated a reduced coating growth with increasing pressures. Further measurements with ZnCl2 were performed to check whether an electrochemical mechanism is involved in the coating process.

MM 26.49 Tue 14:45 Poster C

Hydrogen absorption in Gd thin films and islands — •Sara Wanjelik, Georg Oeltzschner, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

The absorption process of hydrogen in thin Gd(0001) films deposited on a W(110) substrate has been investigated by means of scanning tunneling microscopy (STM) and spectroscopy (STS). The adsorption as the previous step is imaged using the fact that clean and well-ordered Gd surfaces exhibit a highly localized surface state near the Fermi edge which is suppressed due to the adsorption of hydrogen. The surface state reappears after the subsequent diffusion of hydrogen into the bulk material. Thus, we are able to observe the temporal development of the absorption process.

In this contribution we will discuss the absorption behaviour for different layer thicknesses to determine the influence of the respective bulk material because the creation of GdH_2 results in a lattice expansion of about 14%. Due to the adherence of the film on the substrate this expansion occurs only in the perpendicular direction. This is different for free standing nanoislands which are only clamped at the interface. Thus, investigations concerning the absorption behavior are also performed on the size dependence of Gd islands to compare these results with those from thin films.

MM 26.50 Tue 14:45 Poster C

Properties and stability of hydrogen sensors based on magnesium-iron thin films — •Gunther Haas, Jennifer Stiebich, Andreas Laufer, Marc Dietrich, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Thin magnesium-iron films, capped by a catalytic Pd layer, were prepared by RF diode sputtering. Upon exposure to hydrogen the films show reversible changes in the optical reflection and electrical resistivity. These switching effects can be use to detect hydrogen gas. We investigated the influence of the sputter parameters and the layer thickness on the sensor performance in air and argon atmosphere. Due to the layer optimisation the sensitivity could be extended from 4% to less than 1000 ppm hydrogen in air and response times faster then 10 s were obtained. Considering the stability and durability of the sensors, the long-term stability is restricted by the interdiffusion of Mg into the Pd layer and fractional oxidation. Therefore we investigated the effect of an additional metal layer which allows hydrogen diffusion but suppresses the oxidation and/or the interdiffusion of Mg.

MM 26.51 Tue 14:45 Poster C

Chemical trends of the solution enthalpy of hydrogen in 3d transition metals in dilute limit, derived from first principles — •Ugur Aydin[1], Lars Ismer[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung GmbH — [2]University of California, Santa Barbara

Hydrogen embrittlement is a general phenomenon, which has already been observed in several transition metals and which is of high technological relevance. Despite many investigations of related mechanisms, a purely theoretical prediction how much a material of a certain chemical composition is affected by hydrogen embrittlement is still not possible. However, there is no doubt that the hydrogen solution enthalpy, ΔH, and its dependence on the crystal strain is a decisive criterion. We therefore performed a detailed ab initio investigation of the ΔH dependence on the band filling in 3d transition metals under comparable conditions. For this purpose, density functional theory within the GGA approximation was employed. Zero point vibrations have been taken into account using the Einstein model. The analysis revealed a universal dependence on the crystal lattice constant, with a material specific interplay of chemical and strain contributions. We compared our first principles findings with semi-empirical rules for the hydrogen solubility stated by Griessen et *al.* [PRB **38**, 3690 (1988)] and confirmed that out of the parameters discussed there (electronic density, bandwidth of the d-band, atomic spacing) the distance of nearest neighbouring host atoms has the most systematic influence on ΔH.

MM 26.52 Tue 14:45 Poster C

Hydrogen absorption behavior of nano-crystalline Mg thin films — •Helmut Takahiro Uchida, Astrid Pundt, and Reiner Kirchheim — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, D-37077, Goettingen, Germany

Hydrogen absorption behavior of nano-crystalline Mg thin films are electrochemically investigated at room temperature. 20nm Pd-capped nanocrystalline Mg films of different thicknesses were prepared in an UHV chamber, by means of ion beam sputter deposition under Ar-atmosphere at the pressure of 2,5*10E-4 mbar. Nano-crystalline Mg films were deposited on Si (100) substrates for P-C-T measurements of hydriding, and on annealed Pd-substrates with thickness of less than 0.25mm for hydrogen permeation measurements. All the films were covered by a 20 nm thick layer of Pd in order to prevent oxidation. The influence of loading current density on hydrogenation property were observed by measuring electromotive force (EMF). Diffusion coefficient of hydrogen in nano-crystalline Mg thin films at room temperature are estimated at several hydrogen concentration, and the impact of grain boundary on hydrogenation property is discussed. XRD measurements using a Phillips X-Pert diffractometer with a Co-K alpha radiation were performed before and after hydrogenation in order to check the phase transition and change of texture in the sample.

MM 26.53 Tue 14:45 Poster C

Oxygen and silicon diffusion in mixed cation silicate glasses — •Kirsten Sunder and Hartmut Bracht — Institut für Materialphysik, Wilhelm-Klemm-Straße 10, WWU Münster

The impact of alkali (A) and alkaline-earth (M) ions on oxygen (O) and silicon (Si) diffusion in mixed cation silicate glasses of the composition aA2O-bMO-4SiO2 was investigated. In particular, the dependence of network former diffusion on the type of cations (A=Li,Na,K; M=Mg,Ca,K), the concentration of non-bridging oxygens (a=0.5,1,1.25; b=2a), and the alkali to alkaline-earth ratio (a=0,1,1.5; b=3-a) was determined. This study together with the work on the cation mobility [F.V. Natrup et al., Solid State Ionics 180 (2009) p. 109] provides a comprehensive understanding of the dynamics in this glass system.

MM 26.54 Tue 14:45 Poster C

Alternative contacting concept for ZnO nanostructures with regard to sensing applications — •Martin Gnauck[1], Ulrich Schröder[1], Raphael Niepelt[1], Carsten Ronning[1], and Rainer Adelung[2] — [1]Institute for Solid State Physics, Friedrich-Schiller-University Jena — [2]Institute for Materials Science - Functional Nanomaterials, Christian-Albrechts-University Kiel

Due to the direct band gap of 3.37 eV at room temperature and high surface-to-volume-ratios zinc oxide nanowires exhibit some promising properties for upcoming sensing applications. Studying the electrical and opto-electrical properties of single nanowires usually requires complex techniques like electron beam lithography or preparation via focused ion beam (FIB). Well established photolithography, however, is economically reasonable and allows fabrication of new nanostructure based devices on a much larger scale.

Here, we present a comparatively easy method for contacting one- and two-dimensional ZnO nanostructures and investigate their electrical properties with regard to possible applications as UV-light and gas detectors. Therefore, photolithography is used for pre-structuring and pre-contacting the VLS-grown nanowires and nanosails.

MM 26.55 Tue 14:45 Poster C

Polymer-Based Magnetoelectric Composites — •Kerstin Meurisch, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — Technische Fakultät, Institut für Materialwissenschaft, CAU Kiel

In magnetoelectric (ME) materials the change of an external magnetic field induces a change of the internal electric potential. Composites containing a magnetostrictive phase embedded into a piezoelectric matrix exhibit very high indirect ME coefficients compared to those direct ones of single phase materials. Furthermore, using piezoelectric polymers as matrices is advantageous, for example if high flexibility of the product is required or if the product is very sensitive to leakage currents in the matrix. Since polymers generally have a very small dielectric constant and a low Young's modulus, their ME coefficients exceed those of ceramic-based composites. Regarding the design of the composites, several microstructures are possible. The most prominent designs are laminates and particulate structures. Two approaches for the development of an polymer-based ME composite are presented: Firstly, as a basic step towards particulate composites, piezoelectric thin films of Nylon-11 were deposited via thermal evaporation. Secondly, laminates were fabricated by sputtering Cobalt onto a purchased piezoelectric Polyvinylidenfluorid(PVDF) foil. Preliminary results such as the effective piezoelectric coefficient of Nylon-11 and the effective ME coefficient of the laminates will be discussed.

MM 26.56 Tue 14:45 Poster C

Vapour phase deposition of ceramic-based granular nanocomposites for magnetoelectric applications — •Björn Gojdka, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — University of Kiel, Institute for Materials Science, Kaiserstraße 2, 24143 Kiel

The investigation of magnetoelectric materials has experienced a renaissance during the last decade due to promising new theoretical and experimental results and the technical potential of such materials [1]. However, up to now investigations of magnetoelectric granular nanocomposites, in which magnetostrictive clusters are embedded in a piezoelectric matrix, are scarce [2].

We report on the fabrication of granular magnetoelectric nanocomposites via combined rf and DC magnetron sputtering. Quasi-laminar systems, consisting of alternating layers of piezoelectric ceramic and layers of percolated magnetostrictive clusters were fabricated by tandem-sputtering. The deposition by co-sputtering of a BaTiO3 ferroelectric matrix containing clusters of Co on single-crystal SrTiO3 substrate was studied.

The structure was characterized by XRD. For the analysis of the composition and morphology of the composites TEM and SEM/EDX were utilized.

[1] C.W. Nan et al., Journal of Applied Physics 103, 031101 (2008)

[2] J. H. Park et al, Applied Physics Letters 92, 062908 (2008)

MM 26.57 Tue 14:45 Poster C

Ag-TiO2 nanocomposites for antibacterial and photocatalytic applications — Tomislav Hrkac[1], Venkata Sai Kiran Chakravadhanula[1], Nathalie Wohner[1], Vladimir Zaporojtchenko[1], •Thomas Strunskus[1], Dieter Garbe-Schönberg[2], and Franz Faupel[1] — [1]Institut für Materialwissenschaft-Materialverbunde, Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel — [2]Dept. of Geology/ ICPMS Lab, CAU Kiel, Ludewig-Meyn-Strasse 10, 24118 Kiel

Nanocomposites offer the possibility to combine the antibacterial property of Ag with the photocatalytic activity of TiO$_2$ in one material. Here TiO$_2$-Ag 2D and 3D nanocomposites were prepared by physical vapor deposition techniques allowing to varying many different morphologies. The antibacterial efficiency was studied by monitoring the silver release using ICP-MS. The optical structural properties of the composite was characterized by UV-Vis, XRD, HRTEM and XPS, and the photocatalytic activity was determined by UV illuminated dye photo degradation. Considering the different morphologies the correlation of photocatalytic activity and silver release will be discussed.

MM 26.58 Tue 14:45 Poster C

Experimental Thermodynamics and Phase Relations of New Anode Materials for Li-Ion-Batteries — •Hans Flandorfer, Klaus Richter, and Herbert Ipser — Institut für Anorganische Chemie / Materialchemie, Universität Wien, Wien, Austria

Li-Ion batteries have for long been recognized as an efficient way to store electric energy. For use in traction applications, however, these batteries have to meet several design criteria, such as number of charge/discharge cycles, energy density and safety.

The scope of SPP 1473 *WeNDeLIB* is the systematic investigation of materials interaction between the various materials used for cathode, anode, electrolyte and separators. The constitution of the relevant systems has been recognized as an important issue to understand the performance of the whole assembly.

Our Department has long lasting expertise in the field of phase diagram research and determination of thermodynamic properties. Together with other methods like EMF measurements and isopiestic vapor pressure measurements, all data required for thermodynamic modeling can be generated.

Our group will focus on the purely metallic anode materials. Co-Sn, Ni-Sn, Cu-Sn, and many others have been proposed as suitable materials. Thus, thermodynamics and phase relations of the respective ternary systems (Co,Cu,Ni)-Li-Sn will be investigated.

MM 26.59 Tue 14:45 Poster C

Electrochemical investigation of nanoscaled LiCoO$_2$ from different synthesis processes — •Carsten Jaehne, Christine Täschner, Andreia Ioana Popa, Rüdiger Klingeler, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden

Self-assembled nanoscaled cathode materials promise increased rate performance in Li-ion batteries. We report on the conventional and the microwave assisted hydrothermal synthesis of LiCoO$_2$ nanostructures. We discuss the effect of both synthesis processes as well as of the variation of the process temperatures between 120°C and 200°C and of different precursors on the morphology and electrochemical properties of the resulting material. Our electron microscopy, x-ray diffraction and magnetisation studies provide information about the phase, the morphology and the valency of the Co-ions. Cyclic Voltammetry and Galvanostatic Cycling techniques have been applied to evaluate the electrochemical performance.

MM 26.60 Tue 14:45 Poster C

Magnesium secondary batteries based on V$_2$O$_5$ cathodes — •Wiebke Lohstroh, Philipp Leufke, and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology, Postfach 3640, 76021 Karlsuhe, Germany

The development of high performance, reliable energy storage systems is a mandatory prerequisite if the use of fossil fuels shall be curtailed in mobile and stationary applications. Important parameters for any energy storage system are energy and power density as well as reliability, cycle life, safety and cost. Lithium ion secondary batteries are thought to be able to meet these demands and research activities have been intensified in recent years. An alternative pathway, which has only been explored little so far, is a secondary battery based on polyvalent ions,e.g. the Mg/Mg^{2+} redox couple. Mg is abundant and it is thought to be intrinsically safer than the Li analogue thus Mg based batteries could be a viable option for cost sensitive areas.

We will present first results on Mg secondary battery cells using a V_2O_5 cathode, Mg-metal anode and an organometallic electrolyte [1]. V_2O_5 electrodes made from powder show a reversible electrochemical response at potentials between 0 and 2 V vs Mg. However CV measurements indicate that discharge (i.e. Mg intercalation) occurs quite sluggish while during charging two distinct steps can be discriminated. First results on the electrochemical behavior of thin film V_2O_5 electrodes will also be presented.

[1] D. Aurbach, Z. Lu, A. Schechter, Y. Gofer, H. Gizbar, R. Turgeman, Y. Cohen, M. Moshkovich, and E. Levi, Nature 407, 724 (2000).

MM 26.61 Tue 14:45 Poster C

Blends of LiMn2O4 Spinel and LiNi0.8Co0.15Al0.05O2 for Advanced Lithium-Ion Batteries — •Hai-Yen Tran, Corina Täubert, Peter Axmann, and Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Helmholtzstrasse 8, D-89081 Ulm

Lithium manganese oxide spinel is a promising material for the positive electrode in lithium ion batteries due to the high abundance, low cost, non-toxicity, low irreversible capacity loss and high thermal stability. However, it suffers from relatively low discharge capacity, poor cycle life and poor electrochemical performance at elevated temperatures. Therefore, an interesting alternative would be to mix LiNi0.8Co0.15Al0.05O2 (NCA)and lithium manganese oxide spinel in defined ratios in order to compensate for their disadvantages each other. The aim is to obtain a material that could be comparable or even better than the conventional LiCoO2 with respect to discharge capacity, thermal stability and rate capability. In the present work we have evaluated the electrochemical performance of the mixed oxide electrodes by means of galvanostatic cycling with potential limitation. Blending the layered oxide (NCA) with manganese oxide spinel decreased the irreversible capacity loss and at the same time improved the rate capability of the electrodes. In addition, the manganese dissolution from the spinel structure was drastically reduced by NCA blending as well. The experimental results were compared to the theoretical calculations. The obtained results will be presented and discussed during the meeting.

MM 26.62 Tue 14:45 Poster C

Structure and negative thermal expansion in Cu(In1-xGax)(S, Se)2 — •Christiane Stephan[1], Susan Schorr[2], Denis Sheptyakov[3], and Hans-Werner Schock[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Solarenergieforschung, Glienicker Straße 100, 14109 Berlin — [2]Freie Universität Berlin, Fachbereich Geowissenschaften, Malteserstraße 74-100, 12249 Berlin — [3]Laboratory for Neutron Scattering, ETH Zürich & PSI Villigen, CH-5232 Villigen, Schweiz

Compound semiconductors like Cu(In1-xGax)(S, Se)2 are due to their superior optical and electronical properties successfully used as absorber layers in thin film solar cells. These compounds adopt the chalcopyrite type structure, which is characterized by a tetrahedrally coordination of the cations by anions and vice versa. One of the most intriguing properties of solids whose crystal structures are based on tetrahedrally coordinated ions is their negative thermal expansion. To verify this concept, in-situ neutron diffraction experiments in a temperature range from 290K to 1.5K were performed on Cu(In1-xGax)(S, Se)2 powder samples. The lattice parameters and linear thermal expansion coefficients were determined by Rietveld-Analysis of the neutron diffraction data applying the chalcopyrite structure as structural model and using the FullProf suite software package. Negative thermal expansion coefficients were observed for the Cu(In1-xGax)Se2 compounds, whereas the critical temperature, where alpha(a,c) becomes negative, varies with chemical composition.

MM 26.63 Tue 14:45 Poster C

Electrical properties of grain boundaries in Cu(In,Ga)(S,Se)$_2$ thin films for solar cells — •Jaison Kavalakkatt, Daniel Abou-Ras, Melanie Nichterwitz, Raquel Caballero, Björn Marsen, Thorsten Rissom, Thomas Unold, and Hans-Werner Schock — Helmholtz Center Berlin for Materials and Energy, Berlin, Germany

Electron-beam-induced current (EBIC) and electron backscatter diffraction (EBSD) in a scanning electron microscope are powerful tools to investigate the electrical and microstructural properties of grains and grain boundaries in Cu(In,Ga)(S,Se)$_2$ absorber layers in thin-film solar cells. For the present investigation, the Mo/glass stack was stripped off the remaining Cu(In,Ga)(S,Se)$_2$/CdS/ZnO heterojunction, in order to prepare a Cu(In,Ga)(S,Se)$_2$ surface with reduced roughness, leading to both, high-quality EBSD patterns and decreased number of topography artefacts in EBIC distribution images. In comparison to EBIC analyses on cross-section samples, the measurements on back-surfaces increase the number of accessible grain boundaries and therefore improve the statistics of their electrical properties. EBSD maps identify clearly the positions of the grain boundaries as well as allow for their classifications. Across various grain boundaries, profiles were extracted from EBIC distribution images. Corresponding simulation of these profiles provide values for minority-carrier diffusion lengths and recombination velocities at grain boundaries. The general result for Cu(In,Ga)Se$_2$ layers with various In/Ga ratios as well as Cu concentrations is a similar collection at grain interiors and $\Sigma 3$ grain boundaries and a reduced charge-carrier collection at non-$\Sigma 3$ grain boundaries.

MM 26.64 Tue 14:45 Poster C

Efficient simulation of plasmonic structures for thin film silicon solar cells — •Daniel Lockau[1,2], Sven Burger[2,3], Lin Zschiedrich[2,3], Frank Schmidt[2,3], and Bernd Rech[1] — [1]Helmholtz–Zentrum Berlin, Berlin, Germany — [2]Zuse–Institut Berlin, Berlin, Germany — [3]JCMwave GmbH, Berlin, Germany

Thin film silicon solar cells suffer from the disadvantage of a low absorption coefficient of silicon in important spectral regions. In the case of a flat multilayer cell layout a considerable part of the incident light is reflected back out of the cell due to the low absorber thickness. It is therefore desirable to introduce scattering elements that prolong the average photon path length inside the solar cell's absorber. Plasmonic structures are an upcoming area of research in this field. They might be better suited for optimization than other means of light trapping. The influences of periodic arrays of metal scatters on cell absorption can be very well assessed by different simulation methods.

We employ the finite element method for 3D simulations of Maxwell's equations. The setup for our simulations has been proposed by Rockstuhl et al. (C. Rockstuhl, S. Fahr, F. Lederer, *J. Appl. Phys.* 104, 123102 (2008)) who numerically studied absorption enhancement in a thin bulk of amorphous silicon due to scattering on a periodic array of silver discs. Using the same setup we show that our method is very time and memory efficient for the simulation of such plasmonic structures. Absorption enhancement is shown for wavelengths above 500 nm compared to the absorption without silver discs.

MM 26.65 Tue 14:45 Poster C

Structural characterization of AgGaSe$_2$ thin films grown by Chemical Close Spaced Vapor Transport (CCSVT) — •Christoph Merschjann[1], Barys Korzun[1,2], Susan Schorr[3], Thomas Schedel-Niedrig[1], and Martha Christina Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus — [3]Free University Berlin, Institute of Geological Sciences, Berlin, Germany

Thin films ($d \approx 3$ μm) of n-type AgGaSe$_2$ thin films were successfully grown on glass and glass/molybdenum substrates using the technique of Chemical Close Spaced Vapor Transport (CCSVT). The structural characterization of the thin films was carried out by grazing incidence X-ray diffraction (GIXRD). The observed Bragg peaks belong exclusively to the chalcopyrite type structure. The lattice parameters and the atomic position of the anions were determined by Rietveld analysis of the GIXRD data. The structural refinement revealed also, that in the thin film only one phase, chalcopyrite type AgGaSe$_2$, is present.

The results are compared to those published for single crystalline AgGaSe$_2$. A comparative discussion of structural properties of chalcopyrite type compounds with different monovalent cations (Ag$^+$ vs. Cu$^+$) will round the presentation.

MM 26.66 Tue 14:45 Poster C

The Influence of wet-chemical smoothing on electronic properties of Si/SiO$_2$ interfaces prepared by UHV plasma oxidation — •Orman Gref, Bert Stegemann, Enno Malguth, Maurizio Roczen, Heike Angermann, and Manfred Schmidt — Silicon Photovoltaics, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The successful application Si/SiO$_2$ interfaces for ultrathin oxides or nanostructures in third generation photovoltaics requires a minimum density of Si gap states. In order to achieve this goal, the influence of various wet-chemical pre-treatment procedures on the electronic properties of Si/SiO$_2$ interface was investigated. Structurally abrupt Si/SiO$_2$ interfaces were prepared under ultrahigh vacuum conditions by RF plasma oxidation of n-type Si(111) substrates with thermalized neutral oxygen atoms. A decrease the interface states was achieved by saturating dangling bonds through in situ RF hydrogen plasma passivation . The density of gap states at the Si surface and Si/SiO$_2$ interface was investigated by non-destructive and surface-sensitive surface photovoltage (SPV) experiments. Various sequences of wet-chemical oxidation and oxide removal steps in HF- or NH$_4$F solutions were successfully applied to reduce the substrate surface micro-roughness and surface state density. These optimised wet-chemical smoothing procedures yield a significant decrease in interface state densities of the subsequently prepared Si/SiO$_2$ interfaces D$_{it}$=1*10$_{12}$cm^{-2}eV^{-1}, compared to D$_{it}$=3.5*10^{12}cm^{-2}eV^{-1}, obtained after applying solely the standard RCA cleaning process and HF solution.

MM 26.67 Tue 14:45 Poster C

Minority carrier lifetime of InGaAsP and InGaAs absorbers for low bandgap tandem solar cells — •Nadine Szabó, B. Erol Sagol, Ulf Seidel, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Hahn-Meitner-Platz 1 14109 Berlin

At present, III-V triple junction (3J) solar cells are achieving the highest conversion efficiencies (η=41.6%) worldwide. To improve the efficiency significantly, it is necessary to increase the number of junctions and to involve a subcell with an absorber layer in the band gap range of 1eV. We show on the example of the low band gap tandem cell how the choice of the materials, the quality of the bulk, the optimization of the band gap energies and the preparation of the critical interfaces are essential to build a high efficiency solar cell. A four-junction device can be realized by mechanically stacking of a GaAs-based GaInP/GaAs tandem cell with a InP-based InGaAsP/InGaAs tandem cell. We have grown InGaAsP and InGaAs layers lattice matched to InP substrates, and investigated the properties of the absorber bulk material. We will present time resolved photoluminescence measurements of low band gap InGaAs and InGaAsP double hetero structures (DHS). This technique is both sensitive for the quality of the bulk material within the DHS as well as for the interface preparation between barrier and bulk.

MM 26.68 Tue 14:45 Poster C

Electrical characterisation of oxide-pn-junctions under illumination — •Gesine Saucke[1], Benedikt Ifland[1], Constanze Thees[1], Jonas Norpoth[1], Jörg Hoffmann[1], Yimei Zhu[2], and Christian Jooss[1] — [1]Institute of Materials Physics, University of Göttingen, Germany — [2]Brookhaven National Laboratory, Upton NY, USA

Correlation effects in complex oxide materials should strongly affect the properties of a pn-junction with respect to energy conversion under illumination. As a model system of a photo-active oxide junction, epitaxial thin films of p-type Pr$_{1-x}$Ca$_x$MnO$_3$ (PCMO) were deposited on Nb doped SrTiO$_3$ (Nb-STO) single crystals. Low-resistance ohmic contacts on Nb-STO were obtained for deposited Ti or Al top layers, whereas high work function noble metals reveal non-linear IV characteristics. Since correlation effects, e.g. charge ordering in PCMO, takes place at lower temperatures, the electric characterization with and without illumination via IV curves was performed in a temperature range between 10 K and room temperature. A detailed characterization with respect to crystallographic structure, surface morphology, and interface intermixing was performed by means of TEM, AFM, SIMS and EELS. We found a small Ti-Mn exchange at the PCMO/Nb-STO interface which extends over a few lattice cells. In addition, we will present first results on p-type La$_{1-x}$Sr$_x$MnO$_3$ (LSMO) / Nb-STO based cells.

MM 26.69 Tue 14:45 Poster C

Comparative analysis of models for solute trapping in rapid solidification — •Ekaterina Abramova[1], Denis Danilov[2], Peter Galenko[3], Dieter Herlach[3], and Vladimir Lebedev[1] — [1]Udmurt State University, Faculty of Physics and Energetics, 426034 Izhevsk, Russia — [2]Karlsruher Institut für Technologie (KIT), Theoretische Biophysik, 76131 Karlsruhe — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Phase-field models (WBM- and EFKP-model [1,2]) are extended in the present work to rapid solidification in which local non-equilibrium phenomena occur in bulk phases and within the diffuse solid-liquid interface. The extended model is developed using a thermodynamic approach to fast phase transitions within a diffuse interface in a binary system [3]. We investigate solute trapping, which has been introduced to define the processes of non-equilibrium solute redistribution at the solid-liquid interface. The solute trapping effect in solidifying binary melts is compared with previous sharp-interface models and using the present extensions of WBM- and EFKP- phase-field models. This work is supported by RFBR Nos. 08-02-91957NNIO_a, 09-02-12110-ofi-m; ROSNAUKA No. 2009-1.5-507-007-002; DAAD No. A/08/81583; DFG No. HE 1601/19; DLR Agency under contract number 50WM0736.

[1] A.A. Wheeler, W.J. Boettinger, G.B. McFadden: Phys. Rev. E 47 (1993) 1893. [2] B. Echebaria, R. Folch, A. Karma, M. Plapp: Phys. Rev. E 70 (2004) 061604. [3] P. Galenko, D. Jou: Phys. Rev. E 71 (2005) 046125.

MM 26.70 Tue 14:45 Poster C

A phase-field model for polycrystalline grain growth on thin films — •Christian Mennerich, Frank Wendler, and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Polycrystalline grain growth on thin films is of high interest for catalytic active supports or molecular sieves (e.g. zeolites of the MFI-type). Growth competition between the grains determines the final structure of the film and therefore its properties. It is essential to understand the basic principles controlling the selection mechanisms. A phase-field model is presented to describe competitive grain growth on thin films in 2D and 3D. The model is derived from a free energy functional of Ginzburg-Landau type and supports different anisotropy functions to represent various crystal symmetries. The anisotropy is based either on surface energetic or kinetic considerations. As an example, we show results from coffin shaped crystal structures with a fixed aspect ratio competing on thin films. We focus on mechanisms related to the deviation of grain orientations from the film normal. This leads to the outgrowth and extinction of disadvantageously oriented grains, depending on their neighbourhood.

MM 26.71 Tue 14:45 Poster C

Anti-coarsening and complex dynamics of step bunches on vicinal surfaces during sublimation — •Marian Ivanov[1], Vladislav Popkov[2], and Joachim Krug[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str.77, D-50937 Köln — [2]Interdisziplinäres Zentrum für Komplexe Systeme, Rheinische Friedrich-Wilhelms-Universität Bonn, Römerstraße 164, D-53117 Bonn

Using morphological instabilities one can produce templates for nanoscale technology. One example of such an instability is step bunching, which splits a regular vicinal surface into regions of low and high density of monoatomic steps. The dynamics of the surface is described by the Burton-Cabrera-Frank model with boundary conditions provided by mass conservation at the steps. We consider a one-dimensional step train evolving in the presence of sublimation, step-step interactions and an Ehrlich-Schwoebel effect. We show that the interplay of sublimation and step-step interactions removes the conservation law for the crystal volume in the co-moving frame, which has been assumed in previous work [1,2]. As a consequence large step bunches are found to break up into smaller bunches of a characteristic size, and the monotonic coarsening dynamics of the volume-conserving model is replaced by a complex quasiperiodic pattern.

[1] V. Popkov, J. Krug, Europhys. Lett. 72, 1025 (2005) [2] V. Popkov, J. Krug, Phys. Rev. B 73, 235430 (2006)

MM 26.72 Tue 14:45 Poster C

Growth kinetics and morphology of silicon crystallites synthesized from metallic solution — •Thomas Teubner, Robert Heimburger, Nils Dessmann, Torsten Boeck, and Roberto Fornari — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

The growth of large Si crystallites on amorphous substrates at low temperatures is highly desirable for fabrication of thin film solar cells but it remains a very challenging task. We use a low melting metallic solvent for Si seeding as well as subsequent growth. Supersaturation of solvent droplets for seed generation is reached via influx of Si from vapor and can be controlled by deposition rate. In contrast, expansion of Si seed crystal has been performed in a separate steady state solution growth equipment applying hereby a temperature gradient between vertically stacked feeding source, solvent, and substrate. The temperature difference of about 10 K enables continuous flow of solute towards substrate and thus provides the necessary supersaturation of solution around seed crystals. $\{111\}$ and $\{110\}$ facets are thermodynamically flat at 873 K. Even the experimental supersaturation is not sufficient to provoke kinetic roughness. An estimate of ledge free energy for two-dimensional nuclei suggests that the undercooling necessary for nucleation rates of 1 μm^{-2}s^{-1} is 45 K for $\{111\}$ and 18 K for $\{110\}$ facets. Therefore, two-dimensional nucleation on $\{111\}$ facets seems to be unlikely. The grown $\{111\}$ faceted crystals are often twinned and partly exhibit hopper morphology. The latter can be explained by spreading of steps from apexes and edges and by spatial solute inhomogeneity.

MM 26.73 Tue 14:45 Poster C

Growth of para-hexaphenyl (6P) on silicon oxide by hot wall epitaxy — •Markus Kratzer, Quan Shen, and Christian Teichert — Institute of Physics, University of Leoben, 8700 Leoben, Austria

In the present study, the growth of thin para-hexaphenyl (6P) films on silicon oxide has been investigated. The 6P layers were fabricated by hot wall epitaxy (HWE) at substrate temperatures between room temperature and 490 K. As substrate, a Si(100) wafer covered with native oxide was used. Conventional tapping mode atomic force microscopy (TM-AFM) revealed islands of upright standing 6P molecules in the sub-monolayer regime. Domains of different molecular orientation could be distinguished by transverse shear force microscopy (TSM). The influence of the growth conditions on the domain size and the influence of the domain orientation on the growth of the successive layers have been evaluated. HWE turned out to be an excellent method to grow an almost closed single 6P layer with large domain sizes. Support by the Austrian Science Fund FWF is acknowledged.

MM 26.74 Tue 14:45 Poster C

Bucky ball island morphologies on CaF$_2$: Theory and Experiment — •Martin Körner[1,2], Felix Loske[2,3], Mario Einax[1], Angelika Kühnle[3], and Philipp Maass[1,2] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany — [3]Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany

Self-organized growth of C60 molecules deposited on insulator substrates such as CaF$_2$(111) yield novel types of morphologies: regular triangular double layers as well as strange irregular islands with hexagonal-type shape, double layer rims at the island edges and channels directed towards the interior of the islands. The relative fraction of the two types of morphologies changes with the temperature. We present a theoretical model to predict these morphologies based on a facilitated de-wetting mechanism of C60 molecules in the first layer in the presence of nearby C60 molecules in the second layer. Extensive Kinetic Monte Carlo (KMC) simulations of this model show good agreement with the experimental observations. In particular they support conjectures from experimental findings that the channel structures of the irregular islands form after deposition. The theory moreover provides an explanation for the regular triangular shapes despite absence of epitaxial matching with the substrate lattice. Detailed consideration of the rates for the diffusion and de-wetting processes in connection with scaling arguments allows us to determine effective energy parameters that govern the growth kinetics in this system.

MM 26.75 Tue 14:45 Poster C

Computer tomographic investigation of Ostwald ripening — •Thomas Werz and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Similar to grain growth, Ostwald ripening is a competitive coarsening phenomenon in which larger particles grow at the expense of smaller ones. Improved understanding of Ostwald ripening—in particular, at volume fractions of the coarsening phase above 90%—is crucial to several technological applications, such as aging of multiphase metallic materials and liquid-phase sintering. Although such high volume fractions lie well outside the scope of current analytic modelling, they are feasible to study with modern methods of computer simulation and micro-computed tomography (microCT). Indeed, the latter technique promises to deliver *in situ*, real-time images of Ostwald ripening when carried out with synchrotron radiation. Alternatively, the evolution of sample microstructure can be characterized stepwise by alternating scans in a laboratory microCT at room temperature with *ex situ* anneals to induce coarsening. We have followed such a procedure to obtain 3D datasets of Ostwald ripening as it occurs in semisolid Al-Cu binary alloys. Segmentation of the tomographic reconstructions yields time-dependent maps of particle shapes and sizes that can serve both as starting configurations and as experimental tests for computer simulations of the coarsening process.

MM 26.76 Tue 14:45 Poster C

Is abnormal growth actually the norm in nanocrystalline materials? — •Jules M. Dake, Heiko Paul, and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Nanomaterials may enjoy a privileged place in the fantasies of science-fiction writers, but among researchers studying the phenomenon of grain growth, nanocrystalline specimens suffer from a decidedly dodgy reputation. Not only do they generally contain significant impurity levels (though not necessarily much higher than those of conventional samples, when normalized to the total area of grain boundaries), but experiments designed to pin down characteristic parameters like the growth exponent or activation enthalpy for boundary migration are disappointingly inconsistent. Add to this the suspicion that microstructural entities like triple junctions or quadruple points could modify the kinetics of boundary migration for nanosized grains, and you have a recipe for chaos! To cut through this fog, we carried out a systematic study of isothermal grain growth in nanocrystalline Fe using high-temperature x-ray diffractometry—only to be confronted by indirect evidence for the evolution of grain-size distributions in a manner reminiscent of abnormal grain growth. In order to quantify the microstructural inhomogeneity directly and, thereby, clarify the origins of the x-ray results, we subjected select samples at various stages of annealing to microscopic study using EBSD and TEM. The results indicate that it will not be easy to pin the blame for abnormal growth in nanocrystalline Fe on the usual suspects, like precipitates or texture effects.

MM 26.77 Tue 14:45 Poster C

Segregation stabilization of nanocrystalline binary alloys at low solute concentrations — •Lionel Kroner and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Although enhanced properties are predicted for the nanocrystalline state of many materials, the technological exploitation of such improvements generally requires long-term stability of the microstructure at room temperature and short-term stability during processing (e.g. hot pressing, if highly dense bulk samples must be produced from powders). Therefore, effective strategies must be developed to suppress the strong driving force for grain growth that is always present in nanocrystalline materials owing to the very small average grain size. The deliberate addition of an atomic species that segregates to the grain boundaries has already been shown to impart a dramatic improvement in the thermal stability of nanocrystalline Pd powders alloyed with Zr [1]. Can this approach be extended to other materials systems? To answer this question, we prepared a variety of Ni-based and Fe-based nanocrystalline alloys by ball milling elemental powders with small amounts of Zr, Ti, Mo or Co. The higher the segregation tendency, the stronger we expect the inhibiting effect of the solute species to become on grain growth. Using x-ray diffraction, we tested this hypothesis by examining the thermal stability of the samples as a function of annealing temperature, solute concentration and enthalpy of segregation.

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

MM 26.78 Tue 14:45 Poster C

Layer growth of perovskites: computing surface structure and energy barriers as a prerequisite for KMC calculations — •Petar Petrov[1], Hannes Guhl[1,2], and Wolfram Miller[1] — [1]Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin — [2]Fritz-Haber-Institut der Max-Planck Gesellschaft, Faradayweg 4-6, 14195 Berlin

Growing smooth perovskite thin films is the basis of utilizing their promising piezo- and ferroelectric properties in technical applications. In order to understand the deposition processes on atomistic scale kinetic Monte-Carlo (KMC) simulations have been started [1]. However, the activation energies for the relevant surface processes have to be provided by other calculations. The most accurate source are density functional theory calculations, which we have performed for oxygen and hydrogen atoms as well as for water molecules (for oxygen see [2]). On the other hand, the complexity of the problem involving the calculation of many energetic barriers prohibits an in-depth DFT-study of the entire growth process. Therefore, we also use force-field methods based on classical potentials in order to obtain energy barriers for more complex situations within a reasonable time. Potential parameters are adjusted to the results of the DFT calculations and empirical data available in literature.

[1] Petar Petrov, Hannes Guhl and Wolfram Miller, phys. stat. sol. b **245** (2008), 2649

[2] Hannes Guhl, Wolfram Miller and Karsten Reuter, Surf. Sci. (2009) in press

MM 26.79 Tue 14:45 Poster C

Self-organized growth of helicenes on calcite (104) surfaces: Monte Carlo Simulations and Experiments — •Tobias Richter[1], Philipp Rahe[2], Markus Nimmrich[2], Mario Einax[1], Martin Körner[1,3], Angelika Kühnle[2], and Philipp Maass[1,3] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [3]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

Helicene molecules deposited on calcite(104) substrates form one-dimensional double-strands along the [010] direction of the (104) surface. These effectively one-dimensional morphologies show a particular ripening process in the post-nucleation regime due to strong anisotropic diffusion. Kinetic Monte Carlo simulations and extensions of mean-field rate equations are presented to model the increase of the mean chain length of the helicene clusters in dependence of the annealing time. The ripening process exhibits two characteristic time regimes in agreement with the experimental observations.

MM 26.80 Tue 14:45 Poster C

Molecular dynamics simulations of ion transport at the crystal-melt interface during the crystallization of superionic calcium fluoride — •Detlef Stock and Peter Görnert — INNOVENT e.V., Prüssingstr. 27B, D-07745 Jena, Germany

The crystallization of superionic conductors such as calcium fluoride from the melt shows a peculiarity which is due to the liquid-like mobility of anions in the crystalline phase. To understand the atomistic mechanism of the growth process we peform nonequilibrium molecular dynamics (MD) simulations of isothermal crystal growth of calcium fluoride from its undercooled melt for the low index {100}, {110}, and {111} crystal-melt interfaces. The MD simulations are based on parameterized potentials describing long-range Coulomb and pairwise short range interactions. We investigate the ion transport at the interface in terms of ion mobility and average coordination number of the ions as a function of the distance to the interface. As a result we observe the freezing of the cation sublattice, whereas there is only a slight decrease of the anion mobility in the growing crystal. Finally, a comparison of the growth kinetics of superionic calcium fluoride with results for simple fcc metals will be given.

MM 26.81 Tue 14:45 Poster C

Numerical studies on grain growth of Si: Influence of surface energy anisotropy — •Giordano Cantù and Wolfram Miller — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin

With the developing market for multi-crystalline Si dedicated for photovoltaic applications the interest in understanding the details of the grain growth has increased. First numerical simulations on grain growth of Si have been performed by I. Steinbach [1] and detailed experimental investigations have been performed in the group of K. Nakajima (e.g. [2]). Corresponding (2D) calculations to one of the experiments have been performed by Chen *et al.* using a four-fold anisotropy with an anisotropy of 25% [3]. We have performed 2D computations of grain growth into an undercooled using the phase-field model of Warren *et al.* [4] and different approaches for the anisotropy of the surface energy. The influence of the dependence of the surface stiffness as a function of the crystal orientation on the growth kinetics is discussed.

[1] I. Steinbach, Ein Multi-Phasen-Feld Model für facettiertes Kristalwachstum, PhD thesis, Würzburg 2000

[2] Kozo Fujiwara, Yoshikazu Obinata, Toru Ujihara, Noritaka Usami, Gen Sazaki and Kazuo Nakajima, J. Crystal Growth **266** (2004), 441

[3] P. Chen, Y. L. Tsai and C. W. Lan, Acta Mater. **56** (2008), 4114

[4] J. A. Warren, R. Kobayashi, A. E. Lobkovsky, W. C. Carter, Acta Mater **51** (2003), 6035

MM 26.82 Tue 14:45 Poster C

Morphology of Graphene Layers on Ir(111) Studied by SPA-LEED — •Dennis Meyer, Hichem Hattab, Giriraj Jnawali, Dirk Wall, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Fakultät für Physik und Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany

We used SPA-LEED to investigate the morphology of graphene layers on Ir(111) at different growth temperatures. The decomposition of ethylene at 1040°C results in a highly oriented graphene layer. The LEED pattern solely shows the moiré spots surrounding each Ir(111) integer order spot. These satellites arise from the 10% mismatch between the two hexagonal lattices. Between 600°C and 1000°C we observe in addition a broad distribution of almost randomly oriented graphene domains which cover the majority of the surface. These domains give rise to broad arcs in the LEED pattern. There is no commensurate order with respect to the Ir(111) substrate. Another minority graphene domain is rotated by 30° with respect to the Ir(111) lattice, locks in in registry with the substrate, and gives rise to a sharp spot between the moiré patterns of the ordered phase.

MM 27: HV Viehland

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

Invited Talk MM 27.1 Wed 9:30 H16

Multiferroic Composites — •Dwight Viehland — Virginia Tech, Blacksburg VA USA

Multi-functional materials can respond to more than one external stimulus. One important family of such materials would be those with magnetization-polarization interactions: however, prior searches for such systems with strong exchange have proven elusive. In this talk, we will discuss advances in magnetoelectric materials. Investigations of multi-ferroic behavior will be presented for magnetoelectric (i) laminate composites of piezoelectric and magnetostrictive layers; (ii) self-assembled two phase nanocomposite layers; and (iii) self assembled two phase single grain particles. We will demonstrate that strong interaction can be achieved between the spin and polarization subsystems.

MM 28: Nanostructured Materials I

Time: Wednesday 10:15–11:45 Location: H16

MM 28.1 Wed 10:15 H16

Microstructure and thermodynamics of nanocrystalline NiTi alloy processed by high pressure torsion — •reeti singh[1], harald rösner[1], ruslan z. valiev[2], sergiy divinski[1], and gerhard wilde[1] — [1]Institut für Materialphysik, Westfälische Wihelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149, Münster, Germany — [2]Institute of Physics of Advanced Materials, Ufa State Aviation University, 12 K. Marx Street, 450000 Ufa, Russian Federation

An equiatomic nano-NiTi alloy, deformed by high-pressure torsion (HPT) was investigated. By HPT, almost complete amorphization is obtained in bulk NiTi containing B2 austenite. Crystallization and structural changes during annealing were investigated by differential scanning calorimetry (DSC), X-ray diffraction analysis and transmission electron microscopy (TEM). The DSC signals observed during continuous heating experiments from 323 K to 723 K indicate an unusually large separation between the nucleation and the growth stages. A large variation in the grain size is observed after annealing at 723 K. This behavior is discussed with respect to the nanoscale microstructural heterogeneity after initial deformation processing. The activation energy for grain growth was determined to be 289 kJ/mole. Additional TEM studies reveal amorphous bands sandwiched between crystalline parts after heating at lower temperatures below 623 K, where the atomic mobility is sufficiently low to prevent long-range diffusion. The heat release during annealing in the temperature range from 453 K to 623 K shows an unexpected decrease at 423 K, possibly due to a reverse amorphization, takes place at lower temperatures.

MM 28.2 Wed 10:30 H16

Influence of solutes on the deformation behaviour of nanocrystalline alloys: A molecular dynamics study of PdAu — •Jonathan Schäfer, Alexander Stukowski, and Karsten Albe — FB Materialwissenschaft, TU Darmstadt, Germany

In nanocrystalline (nc) metals various deformation mechanisms like grain boundary sliding and rotation have been identified which are not operational in coarse-grained materials. Moreover, it is well established that the barriers for dislocation emission from grain boundaries are governed by the generalized stacking and twinning fault energies.

While a number of elemental metals have been studied in the past, both in experiment and via computer simulations, little is known on how solutes affect the deformation behaviour of nc-metals.

In this contribution, we present molecular dynamics (MD) simulations of nc PdAu. Model structures are created by the Voronoi tesselation technique and alloyed via a hybrid MD/Monte-Carlo method to determine their structural and chemical equilibrium state. The deformation behavior is analyzed with respect to dislocation activity by employing a novel algorithm for dislocation detection. For comparison, chemically equilibrated and randomly alloyed structures are studied. Our results provide an understanding of the effect of substitutional solutes on the deformation processes in miscible, nanocrystalline alloys.

MM 28.3 Wed 10:45 H16

Absolute concentration of free volumes in nanophase metals prepared by high-pressure torsion — •Bernd Oberdorfer[1], Wolfgang Sprengel[1], Daria Setman[2], Michael Zehetbauer[2], Reinhard Pippan[3], Werner Puff[1], and Roland Würschum[1] — [1]Inst. f. Materialphys., TU Graz, 8010 Graz, Austria — [2]Phys. Nanostrukt. Mater., Fakultät f. Physik, Univ. Wien, Austria — [3]Erich Schmid Institute of Materials Science., Leoben, Austria

This contribution is concerned with the yet unsettled question of absolute concentrations of free volumes in nanocrystalline metals. Despite indications for high concentrations of lattice vacancies and excess volumes in non-equilibrated grain boundaries in these materials, studies by direct and specific methods are scarce. Initial studies to determine the absolute concentration of defects in nanocrystalline metals by time-dependent dilatometry are presented. Bulk nanocrystalline Cu and Fe samples were prepared by high pressure torsion. Length-change measurements with a differential dilatometer show the irreversible annealing of excess free volume $\Delta V/V$ of up to ca. 3×10^{-3} (Fe) or 1×10^{-3} (Cu) upon heating. The annealing behaviour is analyzed by non-isothermal transformation kinetics. The relative contributions of the various types of defects (vacancy agglomerates, dislocations, grain boundaries) with respect to the total excess free volumes are discussed. The dilatometric measurements are compared with studies of positron lifetime spectroscopy and differential scanning calorimetry. Financial support by the FWF Austrian Science Fund is appreciated (project P21009-N20).

MM 28.4 Wed 11:00 H16

Mechanical spectroscopy of nanoparticle-reinforced, electrodeposited ultrafine-grained nickel — •Hans-Rainer Sinning[1], Gabriele Vidrich[2], and Werner Riehemann[2] — [1]Institut für Werkstoffe, Technische Universität Braunschweig — [2]Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal

The grain size of electrodeposited ultrafine-grained nickel can be reduced down to the nanocrystalline range by adding ceramic nanoparticles like Al_2O_3 or SiO_2. Mechanical spectroscopy (vibrating-reed technique at 200–800 Hz) reveals several different elastic and anelastic phenomena, all sensitive to annealing, which can be used to characterise the microstructural state, defects, and thermal stability of these nanocomposites. Preliminary results are shown on recovery effects (structural relaxation: increase of Young's modulus and decrease of elastic energy dissipation in wide ranges of temperature), low-temperature mechanical loss peaks, and on the gradual development of amplitude-dependent damping components and of the magnetoelastic "ΔE effect" during grain coarsening. Differences in the annealing characteristics between these quantities, as well as between Ni samples with and without Al_2O_3 or SiO_2 nanoparticles, respectively, are discussed with respect to underlying relaxation mechanisms and related processes of recovery and grain growth. In particular, in case of Al_2O_3 nanoparticles, two separate anelastic relaxation peaks near 170 and 120 K indicate, respectively, both the incorporation of hydrogen and the thermal generation of dislocations at the Ni/Al_2O_3 interfaces.

MM 28.5 Wed 11:15 H16

Thermal stability and reaction of nanocrystalline Fe/Cr multylayers — •Patrick Stender and Guido Schmitz — Institut für Materialphysik, Münster

Thermal stability and reaction of iron/chromium multilayers are analyzed using 3D atom probe technique. For this purpose, stacks of up to 50 layers of pure iron and pure chromium with a single layer thickness of 12 nm were deposited on blunted tungsten tips by ion beam sputtering. Subsequent isothermal and isochronal annealing sequences were carried out in an UHV furnace to investigate the thermal behaviour of the system. In a last processing step, samples were sharpened to 50 nm radius of curvature by annular milling using the focused ion beam technique. Although a miscibility gap exists between a chromium rich phase and an iron rich phase up to 820 °C, nevertheless a short-ranged mixing at the layer interfaces on the length scale below 2 nanometers is observed, which is interpreted by the Cahn Hilliard thermodynamics of inhomogeneous systems. Most remarkable, in suitable temperature-time windows above 550 °C, atomic transport across the metallic layers appears along 1D pipe geometries. This observation is interpreted by triple line transport in the nanocrystalline microstructure. Segregation and transport properties of the triple lines are determined.

MM 28.6 Wed 11:30 H16

Trouble at the boundary surface: modeling field distortions and atom trajectories in 3D-AP — •Christian Oberdorfer and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

Within the last years atom probe tomography (3D-AP) has seen an impressive progress. Instruments utilizing femtosecond laser pulses to trigger the fundamental field evaporation process and a wide angle detector alignment are state of the art. The progress in instrumentation draws focus to more sophisticated methods for data analysis and interpretation, since it is now possible to analyse materials of poor conductivity (ceramics, glasses and semiconductors).

Measurements of these materials will reveal strong artefacts which originate from their heterogeneous electronic properties. In order to address this problem, a simulation of the field evaporation of such specimens is carried out. The electric field at the surface of a modeled specimen is computed using finite elements. A single surface atom then gets field evaporated and subsequently the trajectory onto a detector like counter-electrode is computed. The described procedure is repeated atom by atom until a certain termination condition is reached. Afterwards the collected data of all of the detector positions is used to carry out a common 3D-AP volume reconstruction. This way a detailed analysis of apparent artefacts is enabled.

Results of this approach for different geometric setups of heterogeneous dielectric/metallic structures (layers, precipitates) will be presented and allow estimation of possible measurement artefacts.

MM 29: Nanostructured Materials II

Time: Wednesday 12:00–13:00 Location: H16

MM 29.1 Wed 12:00 H16

Diffusion-induced recrystallization in Ni/Pd bi-layers — •Michael Kasprzak, Dietmar Baither, and Guido Schmitz — Institut für Materialphysik, WWU Münster, Germany

In size-mismatched thin film interdiffusion couples Diffusion-Induced Recrystallisation (DIR) appears instead of the conventional continuous Fickian atomic transport. The new grains formed during this process reveal characteristic composition levels which are so far not understood.

We study this effect in sputter-deposited Ni/Pd films in order to derive a physical interpretation of the preferred compositions. After heat treatment, transmission electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffractometry show that new grains are indeed formed inside the diffusion zone. Characteristic concentration levels for Ni/Pd are derived from XRD data.

A thermo-mechanic model is presented, which determines the thermo-elastic driving force to grain boundary migration. The model assumes that the gradients of Gibbs free energy of the new grain volume behind and of stressed matrix ahead of the moving grain boundary are equal in local equilibrium. This allows the determination of composition and stress in front of the boundary. Remarkably, just those grains which reveal a composition leading to the maximum possible stress in front of the moving grain boundary dominate the diffusion zone by fastest growth. According to our measurements these stresses are rather high, close to the theoretical maximum strength of the material.

MM 29.2 Wed 12:15 H16

Mechanical testing of infiltrated nanoporous gold — •Eike Epler[1], Burkhard Roos[1], Marcus Jahn[1], Lorenz Holzer[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Uni Göttingen, Germany — [2]EMPA, Dübendorf, Switzerland

Recently, nanoporous (np) metal foams have attracted a lot of interest because of their unusual mechanical, electrical, chemical, and optical properties. The very high strength of np Au foams has been the topic of numerous studies and is attributed to a length scale effect, although the exact strengthening mechanisms are not known. Unfortunately, np Au also shows a very low fracture toughness, comparable to that of concrete. In our investigations, we copy nature and combine a brittle material, in this case the np foam, with a ductile material, in this case a polymer, with the goal of achieving a strong and tough composite. Open cell np gold with a relative density of 30% and ligament diameters of around 30nm has been infiltrated with two types of polymers and the elastic modulus, yield strength and fracture toughness of the composite have been measured using micro-mechanical testing methods in the nanoindenter. Results are compared to the uninfiltrated np structure and the bulk material. Additionally, it is possible to fabricate high quality SEM and TEM samples from the infiltrated material with focused ion beam machining, which was not possible in the uninfiltrated foam due to redeposition. The microscopy allows the defect content and foam morphology before and after deformation to be investigated and reveals that nano-twins play an important role in deformation.

MM 29.3 Wed 12:30 H16

X-ray diffraction studies on pore condensates in silica nanochannels: The interplay of sorption strains, capillary condensation and capillary sublimation phenomena — •Daniel Rau[1], Patrick Huber[1], Sebastian Mörz[1], Wolfram Leitenberger[2], and Rolf Pelster[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Universität Potsdam, Germany

We present investigations on the interplay of capillary condensation, capillary sublimation and sorption strains in molecular assemblies confined in template-grown silica nanochannels (SBA-15). The influence of the spatial restriction on the structure of the pore-condensates as well as the influence of the pore-condensate on the structure of the nanochannel array are investigated by wide- and small-angle x-ray scattering techniques.

MM 29.4 Wed 12:45 H16

Electrochemical tuning of the electrical resistance of nanoporous gold prepared by dealloying — Patrick Wahl[1], •Thomas Traussnig[1], Hai-Jun Jin[2], Stephan Landgraf[3], Jörg Weissmüller[2], and Roland Würschum[1] — [1]Inst. f. Materialphysik, TU Graz, Graz, Austria — [2]Inst. f. Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Inst. f. Physikal. u. Theoret. Chemie, TU 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 (e.g., resistance tuning [1,2]) of metals have been initiated making use of nanocomposites of porous nanophase metals and liquid electrolytes. Triggered by recent findings that the surface stress-charge response of nanoporous gold sensitively depends on adsorbed oxygen [3], the variation of the electrical resistance of nanoporous gold upon electrochemical charging in an aqueous electrolyte is studied. Nanoporous gold is prepared by dealloying. Reversible variations of the resistance up to ca. 50% occur due to the formation of an electro-chemical double layer and the chemical interaction of the electrolyte with the surface (primarily the reversible adsorption of OH/O and desorption of O). The charge-induced variation of the resistance in the various electrochemical regimes is discussed.

[1] M. Sagmeister et al., Phys. Rev. Lett. 96 (2006) 156601; [2] A.K. Mishra et al., J. Appl. Phys. 103 (2008) 094308; [3] Hai-Jun Jin et al., Surface Science 602 (2008) 3588. Financial support by the FWF Austrian Science Fund is appreciated (project S10405-N16).

MM 30: Topical Session Photovoltaic Materials I

Time: Wednesday 10:15–11:30 Location: H4

Topical Talk MM 30.1 Wed 10:15 H4

Solar cell absorbers made from rust ? - Stacked-Elemental-Layer-RTP and corrosion of alloys — •Rainer Hock, Roland Schurr, and Astrid Hölzing — University Erlangen-Nürnberg, Chair for Crystallography and Structural Physics, Staudtstraße 3, D-91058 Erlangen, Germany

Semiconducting absorber materials for thin film photovoltaics like $Cu(In,Ga)(S,Se)_2$ can be crystallised by heating thin metallic films in chalcogenide atmospheres. This process is known under the acronym SEL-RTP (Stacked Elemental Layer - Rapid Thermal Processing). In the initial stages of this process, the metallic films are attacked by sulfur, selenium or both, forming often a variety of metal chalcogenides. We had a 'second look' on the initial stage of SEL-RTP for the fabrication of absorber materials for thin film photovoltaic applications. This first step is the corrosion of the metal alloys in chalcogenide atmospheres. The different view on the fabrication process may allow to learn from a field of scientific research which was driven mainly by the oil and chemical industries in the second half of last century. At that time, the focus was directed on the search for corrosion resistant metal alloys for use in sulfur containing atmospheres or liquids. Through a reversed view, SEL-RTP may be seen as the desired and complete corrosion of thin metallic films. At the end of the corrosion process a polycrystalline thin film, monophase and with the desired material properties is hopefully produced. Controlled corrosion than leads to a functional, e.g. photovoltaically active thin film.

MM 30.2 Wed 10:45 H4

Amorphous / crystalline silicon heterojunctions: Changes of structural and electronic properties upon low-temperature annealing — •Hannes Ner Beushausen, Tim Ferdinand Schulze, and Lars Korte — Silicon Photovoltaics, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Solar cells based on amorphous/crystalline silicon (a-Si:H/c-Si) heterojunctions have gained much attention due to their high conversion efficiency. In order to increase the open circuit voltage V_{oc} of these solar cells, the prime objective is to 'passivate' the a-Si:H/c-Si interface, i.e. to suppress interface recombination of photogenerated charge carriers by saturating recombination-active dangling bonds.

Commonly, thin (3-10nm) undoped, nominally intrinsic (i)a-Si:H interlayers are used to acheive this passivation effect. The presented work discusses the structural and electronic changes induced by low temperature post-deposition annealing of such (i)a-Si:H/c-Si structures.

The microscopic configuration of hydrogen in the thin amorphous layers, as probed by Fourier transform infrared spectroscopy (FTIRS), is linked to the improvement of the passivation and a dramatic increase of effective minority carrier lifetime τ_{eff}. With 10 nm thick undoped a-Si:H layers values up to $\tau_{\text{eff}} > 4.5\,\text{ms}$, corresponding to interface recombination velocities S as low as 2 cm/s, were observed.

MM 30.3 Wed 11:00 H4

Rigorous optical simulation of rough interface light trapping structures in thin film silicon solar cells — •Daniel Lockau[1,2], Sven Burger[2,3], Lin Zschiedrich[2,3], Frank Schmidt[2,3], and Bernd Rech[1] — [1]Helmholtz–Zentrum Berlin, Berlin, Germany — [2]Zuse–Institut Berlin, Berlin, Germany — [3]JCMwave GmbH, Berlin, Germany

Thin film silicon solar cells suffer from the disadvantage of a low absorption coefficient of silicon in important spectral regions. In the case of a flat multilayer cell layout a considerable part of the incident light is reflected back out of the cell due to the low absorber thickness. It is therefore desirable to introduce scattering elements that prolong the average photon path length inside the solar cell's absorber. Rough interfaces between the layers of a solar cell have proven to provide efficient and industrially producible light trapping structures. As the scattering structures and the layer thicknesses are in the order of only a few ten wavelengths coherence effects have to be taken into account in the simulation and optimization of such structures.

We employ the finite element method for rigorous simulation of Maxwell's equations on 2D and 3D geometries to investigate light trapping effects produced by rough interfaces in thin film silicon solar cells. To approximate an extended rough surface we examine the influence of boundary conditions and a finite computational domain size on the absorption. We apply Monte Carlo sampling over sets of surface representations to obtain averaged measurement quantities. Simulations of 2– and 3–dimensional rough surface geometries are compared.

MM 30.4 Wed 11:15 H4

Optical and structural properties of MBE grown silicon nanodots for photovoltaic application — •Maurizio Roczen, Enno Malguth, Orman Gref, and Manfred Schmidt — Helmholtz-Zentrum Berlin, Berlin, Deutschland

Third generation Solar cells are aimed to exceed the Queisser-Shockley Limit of 30 % efficiency for single junction silicon solar cells by utilizing the quantum size effect (QSE). In theory, the bandgap of nanosized silicon structures (< 5 nm) widens with decreasing size. A hetero emitter consisting of silicon nanodots embedded in a SiO_2 matrix could therefore serve as an energy selective contact allowing the extraction of high energy carriers before thermalization takes place. The SiO_2 matrix allows passivation of an adjacent c-Si absorber and of the nanodots themselves. To grow crystalline silicon nanostructures of the required size, amorphous silicon nano layers were deposited onto plasma oxidized Si-wafers and silica substrates by e-beam evaporation at ultra high vacuum. Annealing the samples above 620 °C leads to the formation of separate crystalline spheres. Both atomic force and scanning electron microscopy show a clear tendency of decreasing sphere size for thinner primal layers. Crystallinity is confirmed by Raman experiments. To observe the quantum size effect, absorption and photo luminescence measurements were carried out as well as surface photo voltage measurements to check the density of states at the interface. Recent results on doped nanodots are discussed.

MM 31: Topical Session Photovoltaic Materials II

Time: Wednesday 11:45–13:15 Location: H4

MM 31.1 Wed 11:45 H4

The influence of reducing the chalcogen to metal ratio on phase transitions during the crystallisation of photovoltaic materials CuIn(S,Se)2 — •Astrid Hölzing[1], Roland Schurr[1], Stefan Jost[2], Jörg Palm[2], Barbara Tautz[3], Felix Oehlschläger[3], Ulrike Künecke[3], Klaus Deseler[3], Peter Wellmann[3], and Rainer Hock[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, FAU, Erlangen, Deutschland — [2]Avancis GmbH & Co. KG, München, Deutschland — [3]Materials for Electronics and Energy Technology, FAU, Erlangen, Deutschland

Time resolved monitoring of the crystallisation of the thin film absorber materials CuIn(S,Se)2 while annealing stacked elemental layers (SEL) yields phase transitions proceeding during the chalcopyrite synthesis. In-situ XRD and DSC measurements on similar processed precursors provide complementary information on intermediate phases and the reaction kinetics of the chalcopyrite formation can be obtained. Thin layers of metals and chalcogens are deposited onto Mo-coated substrates by DC-magnetron sputtering and thermal evaporation, respectively. The XRD powder diagrams recorded while annealing the SEL are quantitatively analysed by Rietveld refinements. Miscellaneous binary selenides and sulfides as well as ternary sulfoselenides are observed by the chalcogenisation of the intermetallic alloy yielding different educts for the chalcopyrite formation depending on the chalcogen content. The presented study will be focused on the influence of reducing the chalcogen to metal ratio on the processing of photovoltaic materials CuIn(S,Se)2.

MM 31.2 Wed 12:00 H4

Properties of grain boundaries in $Cu(In,Ga)Se_2$ and $Cu(In,Ga)S_2$ thin film solar cells deduced from mean inner coulomb potential measurements — •Sebastian S. Schmidt[1], Daniel Abou-Ras[1], Joachim Klaer[1], Raquel Caballero[1], Christoph T. Koch[2], Thomas Unold[1], and Hans-Werner Schock[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Max Planck Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Polycrystalline $Cu(In,Ga)Se_2$ and $Cu(In,Ga)S_2$ thin films are efficient absorbers in thin film solar cells. The solar cell efficiencies strongly depend on the physical properties of grain boundaries in the absorbers. Here, we investigate the local behavior of the mean inner coulomb potential (MIP) at grain boundaries in $Cu(In,Ga)Se_2$ and $Cu(In,Ga)S_2$ solar cell absorbers. With in-line holography in a transmission electron microscope we measure MIP wells at grain boundaries in both types of absorber layers. The depth of the MIP wells depends on the grain boundary type as well as the composition. Generally, the potential wells have a FWHM of about 1 nm perpendicular to the plane of the grain boundary. Since the Debye length is about 10-40 nm in the absorber layers, considerable excess charge accumulations and related band bending at the analyzed grain boundaries can be excluded. A variation in composition seems to be responsible for the formation of MIP wells at grain boundaries. We discuss the local composition at grain boundaries by utilizing the isolated atom approximation.

MM 31.3 Wed 12:15 H4

Structural and chemical analyses of MOVPE-grown $CuGaSe_2$ layers on (001)-GaAs — •Stefanie Bierwirth[1], Susanne Siebentritt[2], Levent Gütay[2], Jes Larsen[2], and Michael Seibt[1]

— [1]Universität Göttingen — [2]Université du Luxembourg

This contribution has been withdrawn.

MM 31.4 Wed 12:30 H4

Characterisation of thin C60 films using X-Ray methods — •Chris Elschner, Alexandr A. Levin, Christoph Schuenemann, Moritz Riede, and Karl Leo — TU Dresden, Institut für Angewandte Photophysik 01069 Dresden George-Bähr-Straße 1

C60 is a well known and often used molecule for state of the art organic solar cells. To increase the efficiency in these nanoscale systems, it is necessary to control the morphology of the thin film layers with the aim to optimize the electrooptical properties. Thin C60 film layers are produced via vacuum deposition under variation of substrate temperature from 30°C up to 90°C, film thickness from 25 nm to 50 nm, and vacuum chamber pressure. The characterisation of the film layers is carried out using x-ray reflection (XRR) and x-ray diffraction (XRD). From these results, the crystallinity, the film thickness, the roughness, and the density of the film layer can be estimated. Using the Scherrer equation, we estimate the average crystal size, which shows the existence of nanoscale crystals (10 nm) in a 50nm C60 film. These results are the base for the coming investigations of mixed organic layers for the use in organic solar cells.

MM 31.5 Wed 12:45 H4

Effect of film thickness, type of buffer layer, and substrate temperature on the morphology of dicyanovinyl-substituted sexithiophene films — •Alexandr A. Levin[1], Marieta Levichkova[1], Martin Pfeiffer[2], Dirk Hildebrandt[2], David Wynands[1], Chris Elschner[1], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Heliatek GmbH, 01187 Dresden, Germany

Dicyanovinyl-substituted sexithiophenes (DCV6T) are promising photoactive materials [1]. The influence of the film thickness, type of buffer underlayer, and deposition substrate temperature on the morphology of the DCV6T layers is investigated by means of X-ray diffraction and X-ray reflectivity methods. A neat Si wafer or a Si wafer covered by a 15 nm buffer underlayer of fullerene C60 or 9,9-Bis[4-(N,N-bis-biphenyl-4-yl-amino)phenyl]-9H-fluorene (BPAPF) is used as substrate.

The crystalline nature and ordered molecular arrangement of the films are proven down to 6 nm film thickness. With increasing substrate temperature or film thickness, the DCV6T film relaxes, resulting in reducing the interplane distances (from 11.29(5) Å to 10.78(5) Å) closer to the bulk value (10.14(1) Å). Considering the same thickness, the DCV6T film relaxes for growth on Si to BPAPF to C60. Thicker films are characterized by smaller density and higher roughness. A thin (some nm-thick) intermediate layer with linear density-gradient is formed in DCV6T/C60 interface for the films with buffer C60 layer.

[1] D. Wynands et al., J. Appl. Phys. 106 (2009) 054509.

MM 31.6 Wed 13:00 H4

Morphological study of Zinc-Phthalocyanine for organic solar cells — •Christoph Schünemann, Chris Elschner, Alexandr Levin, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Germany

Phthalocyanines (Pc) are well known organic molecules and often used in the photoactive layer of small molecule organic solar cells. Reasons for the wide application of these organic semiconductors are their thermal stability, simple way of deposition and their common use as model system. However, the influence of the morphology on the electrical properties of organic solar cells has been investigated only rudimentary so far. In this work, the crystal structure, the growth and the stacking of Zinc-Pc molecules in thin films are investigated with x-ray diffraction (XRD) and x-ray reflection (XRR) methods. For this purpose, we varied the ZnPc film thickness from 5 nm up to 50 nm and the substrate temperature while deposition from room temperature up to 90 °C. Using XRR and atomic force microscopy, we found that the roughness of ZnPc increases with increasing substrate temperature and layer thickness. The XRD measurements show that the ZnPc layers are polycrystalline for all substrate temperatures and layer thickness. Analysing the XRD pattern we also found out, that the ZnPc films are triclinic and the atomic structure does not change with variation of the deposition parameters. The dislocation density and the microstrain in the ZnPc layer decreases with rising film thickness while the crystallite size is in the range of the layer thickness.

MM 32: Topical Session Multifunctional Materials I

Time: Wednesday 10:15–11:45 Location: H6

Topical Talk MM 32.1 Wed 10:15 H6

Fabrication of TiNi thin film stents — Rodrigo Lima de Miranda, Christiane Zamponi, and •Eckhard Quandt — Kaiserstrasse 2, 24143 Kiel

The success of stents and other medical implants, which conventionally consist of thin walled, laser structured tubes based on superelastic TiNi on the one hand, and the limitations regarding the miniaturization of these medical devices on the other hand, has motivated the application of thin film technology as an attractive alternative approach for some applications, e.g. devices for small vessels.

This work introduce the fabrication and characterization of structured cylindrical TiNi thin films by magnetron sputtering, lithography and wet etching based on previous developments of shape memory alloy films. The TiNi thin films devices fabricated in this work have high potential for application as vascular implants, e.g. stents.

The deposition of TiNi thin films on a cylindrical substrate employs a specific device which allows an in situ rotation of the substrate during the sputtering process. The mechanical properties of the deposited cylindrical TiNi films were tested by tensile testing. Axial and radial directions of the film were tested and both film directions showed comparable mechanical properties with TiNi planar films. Superelastic plateau, closed loop hysteresis and a strain up to 6 % were observed.

Topical Talk MM 32.2 Wed 10:45 H6

First-principles computational design of multifunctional materials — •Arthur Ernst — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Development and engineering of new multifunctional materials is one of the main goals in modern condensed matter physics. Thereby, first-principles simulations play a significant role in the design of new materials. Nowadays ab-initio methods based on density functional theory can provide accurate information on structural, electronic, magnetic, and transport properties of realistic systems and has therefore become a major supplement and alternative to experiment.

The presented results are based on multiple-scattering theory which provides explicitly the Green function, which can be used in many applications such as spectroscopy, transport, and many-body physics. Combined with the coherent-potential approximation, this method can be used as well for the description of alloys and pseudo-alloys.

In the talk I will focus on the electronic, magnetic, and transport properties of complex systems like multiferroics, thin metallic films, and oxide heterostructures. The microscopic origin of magnetic and magnetoelectric coupling via interfaces is discussed. The efficiency of the approach is demonstrated.

MM 32.3 Wed 11:15 H6

Towards elastic ceramics and semiconductors — Yogendra Kumar Mishra, Thomas Preusse, Maria Claus, Charline Wolpert, Sebastian Wille, Sören Kaps, and •Rainer Adelung — Functional Nanomaterials, Institute of Materials Science, CAU Kiel, Germany

Designing a material that is elastic and can withstand high temperatures like 1000 °C or more is difficult to design, as polymers do decompose at lower temperatures and metals tend to melt. Especially under ambient conditions, often oxygen creates a problem for metals at these temperatures. Therefore, the design of a flexible ceramic material is desired. If it is at the same time a semiconductor, it has potential as a multifunctional material. In this presentation, we show how a ceramic material has to be organized to show bulk elasticity. In situ experiments show a semiconducting material bended with a manipulation needle in the scanning electron microscope. Furthermore, all details of the fabrication process and the microanalysis understood so far will be presented discussed.

MM 32.4 Wed 11:30 H6

Nanowire-based sensors for chemical species — •Dawit Gedamu, Maria Kassab, Seid Jebril, and Rainer Adelung — Kaiserstr. 2, 24143 Kiel

ZnO has been given lots of attention as it is promising multifunctional material for various applications because of its large direct band gap of 3.37 eV at room temperature and large exciton binding energy of 60 meV. Change in electrical conductance of ZnO thick film , nanostructures , nanowires is reported when such structures are exposed to different chemical species. In this work, a nanowire of ZnO was chosen since such structure has an immense surface area to volume ratio. A suitable and cost effective approach called thin film fracture approach is used to fabricate the nanowire . Under ambient conditions both thin film and nanowire of ZnO deposited by RF sputtering were found to show electrically insulating behavior. Post annealing above 600 K in ambient condition for about 1 hour however has resulted in electrical conductance in both the thin film and the nanowire. When such a nanowire is exposed to oxygen, it shows a quick variation in the electrical conductance for different oxygen concentrations (pressures). Gold (Au) nanowires produced with such a approach were also studied for bio-sensor application. [1] E. S. Jung et al, phys. stat. sol. (b) 244, 5, 1553 (2007) [2] S. Kim and J. Maier Electr. Sol. Stat. Lett. 6 (11), J7 (2003) [3] Chien-Yuan Lu et al, IEEE SENS. J. 9, 4 (2009) [4] S. Jebril et al. Small 4, 2214 (2008).

MM 33: Topical Session Multifunctional Materials II

Time: Wednesday 12:00–13:00 Location: H6

Topical Talk MM 33.1 Wed 12:00 H6

Strain-dependent ferroic properties of doped LaMO$_3$ (M = Mn or Co) and BiFeO$_3$ — •Kathrin Dörr[1], Diana Rata[1], Andreas Herklotz[1], Orkidia Bilani[1], Martina Dekker[1], Ludwig Schultz[1], Marianne Reibold[2], Michael Biegalski[3], and Hans Christen[3] — [1]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [2]Technische Universität Dresden, Speziallabor Triebenberg, 01328 Dresden, Germany — [3]Oak Ridge National Laboratory, CNMS, PO Box 2008, Bethel Valley Rd.,Oak Ridge, TN 37831, USA

Elastic strain at epitaxially grown interfaces provides an efficient coupling mechanism in two-phase multiferroics: piezoelectric or magnetostrictive strain arising from application of an electric or a magnetic field is transferred readily between the components. We employ a piezoelectric single-crystalline substrate to apply reversible biaxial strain to epitaxially grown magnetic or ferroelectric films and study the strain response of their ferroic properties. The relaxor-based 0.72PbMg$_{1/3}$Nb$_{2/3}$O$_3$ -0.28PbTiO$_3$(001) (PMN-PT) proved to be a favourable piezo-substrate with large, reversible, uniform in-plane strain which shows little temperature dependence. The magnetization vs. strain of doped LaMO$_3$ (M = Mn or Co) phases has been studied. It reveals the impact of the strain-induced tetragonal lattice distortion on the ferromagnetic double exchange and the magnetic moment of Co ions that leads to moderate or large magnetization modulation. Further, the strain dependence of ferroelectric switching has been investigated for multiferroic BiFeO$_3$. It displays a large response of unexpected sign attributed to a strain influence on kinetics.

MM 33.2 Wed 12:30 H6

Riesen-magnetoelektrischer Effekt in dünnen FeCoBSi-AlN Kompositfilmen — •Henry Greve[1], Eric Woltermann[1], Hans-Joachim Quenzer[2], Bernhard Wagner[2] und Eckhard Quandt[1] — [1]Anorganische Funktionsmaterialien, Institut für Materialwissenschaft der Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel — [2]Mikrosystemtechnik, Fraunhofer Institut für Siliziumtechnologie ISIT, Fraunhoferstr. 1, 25524 Itzehoe

Magnetoelektrische (ME) Kompositmaterialien, bestehend aus einer piezoelektrischen und einer magnetostriktiven Phase, haben in letzter Zeit immer mehr an Beachtung gewonnen, da sie um mehrere Größenordnungen höhere ME Koeffizienten aufweisen können als einphasige Materialien. Solche riesen-magnetoelektrischen Komposite sind viel versprechend für Anwendungen wie z.B. hochempfindliche Magnetfeldsensoren. 2-2 Dünnschichtkomposite, bestehend aus AlN und amorphen Fe$_{57}$Co$_{18}$B$_{14}$Si$_1$ Lagen, wurden mittels Magnetronsputtern auf Si (100) Biegebalken abgeschieden. Nach thermischem Auslagern in einem externen Magnetfeld weisen die Komposite einen extrem hohen, direkten ME Koeffizienten von 737 V/cmOe bei der mechanischen Resonanz des Biegeelements von 753 Hz auf. Außerhalb der Resonanz bei 100 Hz beträgt der ME-Koeffizient 3,1 V/cmOe. Dies sind die höchsten bisher erreichten ME Koeffizienten für Dünnschichtkomposite. In Kombination mit der durch Magnetfeldglühung und Formanistropie erzielten magnetischen Anisotropie machen diese einzigartigen Eigenschaften die ME Schichten zu höchst attraktiven Kandidaten für MEMS (Mikroelektromechanische Systeme) basierende Vektorfeldsensoren.

MM 33.3 Wed 12:45 H6

Strain-dependent magnetism of La$_{0.8}$Sr$_{0.2}$CoO$_3$ — •Andreas Herklotz[1], Mike Biegalski[2], Hans Christen[2], Ludwig Schultz[1], and Kathrin Dörr[1] — [1]IFW Dresden, Germany — [2]CNMS, ORNL, USA

Perovskite transition-metal oxides have attracted much attention because of the possibility of tuning the magnetic and electronic properties of thin films through interface effects such as exchange interactions, charge transfer, and epitaxial strain.

We investigate the strain-dependence of epitaxial LSCO (La$_{0.8}$Sr$_{0.2}$CoO$_3$) thin films in two ways. First, we grow LSCO in different strain states on PMN-PT(001) (0.72PbMg$_{1/3}$Nb$_{2/3}$O$_3$-0.28PbTiO$_3$) substrates. Compositionally controlled LASO (LaAl$_{1-x}$Sc$_x$O$_3$) buffer layer serve to allow for a tunable lattice strain not affected by the underlying substrate. Second, we use the ferroelectric PMN-PT substrates to biaxial compress as-grown films reversibly by more than 0.1%.

Our experiments show that biaxial strain suppresses ferromagnetism. We have recorded a decrease in the average Co magnetic moment and the transition temperature with increasing tensile strain from as grown films. The dynamic strain experiments help to gain further insight into phase-separated cobaltites and indicate a domination of the double exchange. A considerable change of the Co spin state cannot be observed.

MM 34: Liquid and Amorphous Metals I

Time: Wednesday 10:15–11:15 Location: H5

MM 34.1 Wed 10:15 H5

Structural Behavior of Cu-based Bulk Metallic Glasses under Compression — •Gang Wang[1], Norbert Mattern[1], Josef Bednarčik[2], Simon Pauly[1], JinMan Park[1], Yue Zhang[1], Jun-Hee Han[1], and Jürgen Eckert[1,3] — [1]Institute of complex materials, IFW-Dresden, 01069 Dresden, germany — [2]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [3]Institute of Materials Science, TU Dresden, D-01062 Dresden, Germany

The structural behavior of Cu-Zr binary bulk metallic glass (BMG) family under stress was investigated by means of in-situ high energy X-ray synchrotron diffraction. The components of the strain tensor were determined from the shifts of the maxima of the structure factor in reciprocal space as well by the atomic pair correlation function (PDF) in real space. The analysis of the PDF versus stress shows the occurrence of changes in short-range orders of the glass during elastic deformation. The number density of Cu-(Zr,Cu) and Zr-Zr nearest-neighbor atomic pairs becomes oriented along the loading direction. During plastic deformation the dominating volume fraction of the BMG exhibits the yield strain. The local deformation in shear bands can not be seen in the volume averaged PDFs. After unloading even in the plastically deformed state, the PDFs are identical to the as-cast state are within the error limits, which suggests that this anisotropic rearrangement of atoms under stress is a reversible process. The contribution of the plastically deformed regions localized within the shear bands are too low and therefore not visible in the diffraction patterns.

MM 34.2 Wed 10:30 H5

Study of structural anisotropy in Zr-Cu bulk metallic glasses under uniaxial compression by computer simulations — •Yue Zhang[1], Norbert Mattern[1], Gang Wang[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Helmholtzstr.20, D-01069 Dresden, Germany — [2]Institute of Materials Science, TU Dresden, D-01062 Dresden, Germany

The atomic structures of Zr35.5Cu64.5 and Zr50Cu50 bulk metallic glasses (BMGs) under uniaxial compression are studied by reverse Monte Carlo (RMC) and molecular dynamic simulations. The data obtained from in-situ high energy synchrotron diffraction were fitted using RMC simulation. The dynamic structural change during uniaxial compression is studied from both the short range order (SRO) and medium range order (MRO) aspects. The structural anisotropy is characterized by performing Voronoi tessellation, common neighbor and Honeycutt-Anderson analyses to the resulting atomic configurations. Finally, the relationship between MRO and the distribution of icosahedra is discussed.

MM 34.3 Wed 10:45 H5

Distribution of oxides in a Zr-Cu-Ni-Al-Nb-Si bulk metallic glass — •Jochen Heinrich[1], Frank Mueller[2], Ralf Busch[1], and Stefan Huefner[2] — [1]Chair of Metallic Materials, Saarland University, PO Box 151150, 66041 Saarbrücken, Germany — [2]Chair of Experimental Physics, Saarland University, PO Box 151150, 66041 Saarbrücken, Germany

The course of oxide presence with distance from the sample surface and bonding partner was studied for the bulk metallic glass with the nominal composition Zr57.9Cu15.4Ni12.7Al10.2Nb2.8Si1 (at%) by X-ray photoelectron spectroscopy (XPS). Investigated specimens are taken from vacuum quench-cast rods subjected to oxidation at room temperature and atmosphere. Binding energies were determined in various depths using ion beam ablation of up to 100 nanometers. XPS spectra confirm oxidation primarily of the pure zirconium and aluminum constituents, all other peaks correspond to metallic bonds. While the surface area shows a passivating zirconia layer a few nanometers thick, oxygen is bonded predominantly with aluminum inside the bulk. Since the concentration of oxygen is a crucial factor in the crystallization behavior of bulk metallic glass forming liquids on basis of oxygen affine metals, so far only high purity materials were thought to be suitable. The findings in this study, however, are promising for alloys with industrial grade elements with sufficient glass forming ability. Comparisons of the alloy with differing oxygen content support the conclusion that aluminum acts as an appropriate scavenger for both adsorbed and large amounts of intrinsic oxygen in zirconium based amorphous metals.

MM 34.4 Wed 11:00 H5

Heterogeneous Gd-Hf-Co-Al metallic glasses by liquid-liquid phase separation — Jun Hee Han[1,2], Norbert Mattern[1], and •Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [2]TU Dresden, Institute of Materials Science, Dresden, Germany

The unique microstructures of phase separated metallic glasses can lead to enhanced properties of materials with its heterogeneity. Phase separated metallic glasses were prepared in Gd-Hf-Co-Al system by rapid quenching of the melt. The compositions were chosen by the combination of Gd-Co-Al and Hf-Co-Al alloys showing high glass forming ability. Strong positive enthalpy of mixing (ΔHmix)between the principal elements Gd and Hf leads to a heterogeneous microstructure of Gd-Hf-Co-Al glassy alloys consisting of two amorphous phases Gd-enriched and Hf-enriched. The length scale of spherical shaped heterogeneities ranges from a few nanometers to tens of micrometers. For clearly phase separated composition with nano-meter scale (˜100nm) secondary phase separation is observed in each amorphous phase. Furthermore, thermal behaviour of Gd-Hf-Co-Al phase separated metallic glasses was investigated in order to analyze the composition dependence of glass transition temperature (Tg) and crystallization temperature (Tx), as well as phase sequences upon heating. Funded by DFG Ma1531/10.

MM 35: Liquid and Amorphous Metals II

Time: Wednesday 11:30–12:30 Location: H5

MM 35.1 Wed 11:30 H5

Effect of microstructure on the mechanical properties of metallic glasses — •Steffen Schmitz, Wolfgang Löser, and Bernd Büchner — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Ordinary bulk metallic glasses (BMG) are characterized by high strength, but are usually very brittle. To combine high strength with some ductility, it is necessary to develop new concepts of alloy designing. Here phase separated metallic glasses are chosen, which involve binary terminal systems with both, negative and positive enthalpy of mixing, whereby the structure consists of two different amorphous phases or of nanocrystalline inclusions in an amorphous matrix. Rods and splats of the BMG model system Cu-Zr-Al with small additions of different elements (Gd, Co or Re) with positive enthalpy of mixing to one of the alloying elements are prepared. Their microstructure and glass forming ability (GFA) in dependence of the sample size are investigated and the consequences for mechanical properties are discussed. The GFA is increased by addition of Gd but reduced by addition of Co or Re. The mechanical properties of the Re containing alloys differ strongly from the other alloys investigated by having higher plastic strain at lower stress.

MM 35.2 Wed 11:45 H5

Glass forming ability of iron based amorphous alloys depending on Mo, Cr and Co content — •Uwe Siegel, Uta Kühn, and Jürgen Eckert — IFW Dresden, PF 27 01 16, D-01171 Dresden

The Fe41Co7Cr15Mo14C15B6Y2 multicomponent Fe-based alloy is known to be one of the best glass formers in iron-based systems and shows a critical casting thickness of 16 mm [1]. The elements constituting the alloy have different influences on the glass forming ability. Therefore, the content of Mo, Cr and Co was systematically changed in the master alloy Fe77-x(Co,Cr,Mo)xC15B6Y2 to investigate how these three elements support the glassy microstructure. It was found that a certain content of Mo, Cr, and Co leads to a microstructure of amorphous matrix and alpha-Fe precipitates without any carbides.

[1] Shen, J., Chen, Q. J., Sun, J. F., Fan, H. B. & Wang, G. Exceptionally high glass-forming ability of an FeCoCrMoCBY alloy. Applied Physics Letters 86, (2005).

MM 35.3 Wed 12:00 H5

Thin amorphous tantalum films: Preparation and properties of samples formed by e-beam evaporators — •Kevin Stella[1], Damian Bürstel[1], Steffen Franzka[1], Oliver Posth[2], and Detlef Diesing[1] — [1]Institut für Physikalische Chemie, Universität Duisburg Essen — [2]Institut für Experimentalphysik, Universität Duisburg Essen

Large area ($A = 6\,\mathrm{cm}^2$), thin tantalum films ($5\,\mathrm{nm} < d < 100\,\mathrm{nm}$) are accomplished by evaporation from tantalum rods using small pocket e-beam evaporators. Using a sample to source distance of ≈ 20 cm, homogeneous amorphous films with a small surface roughness ($< 1\,\mathrm{nm}$) can be prepared on glass. Films are characterized by scanning electron microscope images, atomic force microscopy, electrochemical oxidation and resistivity measurements as function of film thickness. The samples show high resistivities of $200 - 2000\,\mu\Omega\cdot\mathrm{cm}$. The temperature coefficient of the resistivity (TCR) is negative as characteristic for highly disordered metals.

MM 35.4 Wed 12:15 H5

Investigation of $(\mathrm{Cu}_{60}\mathrm{Co}_{40})_{1-x}\mathrm{Zr}_x$ Alloys for Glass Forming Ability and Phase Separation — •Björn Schwarz[1], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, Helmholtzstrasse 20, D-01069 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

CuZr as well as CoZr are well known metallic glass formers in a wide compositional range. Since the binary CuCo systems exhibits a metastable liquid-liquid miscibility gap, i. e. Cu and Co tend to separate from each other, the ternary Cu-Co-Zr system is a promising candidate to form phase separated glass-glass composites. In this work $(Cu_{60}Co_{40})_{1-x}Zr_x$ metallic glasses down to relatively low Zr contents of $x = 32$ could be prepared by melt spinning technique and the as quenched as well as several heat treated states were investigated by x-ray diffraction, dynamical scanning calorimetry, high-resolution transmission electron microscopy, (in-situ) small angle scattering, x-ray photoelectron spectroscopy and magnetization measurements in order to reveal if phase separation is present in the as quenched amorphous state or if it can be induced by thermal treatment.

MM 36: HV Bitzek

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

Invited Talk MM 36.1 Wed 14:00 H16

Atomistic simulations of plastic deformation - insights from a quantitative approach — •Erik Bitzek — Lehrstuhl Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg

Since the first studies on dislocation core structures in the 1960s, atomistic simulations have become an important tool to investigate the mechanical behaviour of materials. Atomistic simulations, for example, allow the direct observation of fundamental dislocation processes like the nucleation of dislocations and their interaction with defects at a length scale where experimental information is difficult to obtain. Besides this kind of *qualitative* studies, atomistic simulations are more and more used in a multiscale modelling framework to provide *quantitative* information on parameters for mesoscopic models like dislocation dynamics simulations. Systematic parameter studies and statistical analysis of atomistic simulations can however provide additional insights, e.g. by revealing correlations between different parameters or by providing a test-bed for (mesoscopic) models.

This talk will provide an overview on parameter studies on dislocations in single crystals, dislocation mediated plasticity in nanocrystals and plastic deformation of metallic glasses by shear transformation zones. The detailed quantitative analyses of the atomistic simulations are compared to current models of nanoscale plasticity.

MM 37: Mechanical Properties II

Time: Wednesday 14:45–16:15 Location: H16

MM 37.1 Wed 14:45 H16

An alternative way to determine Young's modulus of thin films — •Matthias Herrmann and Frank Richter — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

An extension for the original approach of Pharr's and Bolshakov's *effective indenter* concept given by Schwarzer (J. Phys. D: Appl. Phys. 37 (2004) p.2761) allows one to apply linear elastic contact solutions for layered half spaces to actual elastic-plastic indents and, hence, might be taken into account as an alternative way to analyze the elastic response of thin films. In this contribution, it is discussed to what extent the *effective indenter* concept can be used to determine Young's modulus of a thin film. Therefore, a thermally grown SiO_2 film and *a*-C:H films deposited by PECVD were exemplarily used. For each sample, elastic-plastic load-depth curves (Berkovich) for a series of varying maximum loads were analyzed in order to realize the *effective indenter* approach for data of varying contact depth to film thickness ratio. The modulus values obtained in this way were in reasonable agreement to those obtained by elastic spherical indentations if the contact depth to film thickness ratio was sufficiently low. Physical mechanisms are discussed as reasons for the deviation obtained at higher contact depths.

MM 37.2 Wed 15:00 H16

Creep measurements on ultra-fine grained copper after high-pressure torsion straining — •Jörn Leuthold[1], M. Wegner[1], S. Divinski[1], K. A. Padmanabhan[1], D. Setman[2], M. Zehetbauer[2], and G. Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Germany — [2]Fakultät für Physik, Universität Wien, Austria

Ultrafine grained materials, especially such materials that have been processed by severe plastic deformation under a high hydrostatic pressure, present unique properties such as an increase in yield strength and simultaneously a considerable uniform tensile elongation before failure. 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. Grain boundary controlled mechanisms, such as grain boundary emitted dislocations and partial dislocations, twinning, grain boundary diffusion and sliding can be more important or even dominant. To study the deformation behavior, several copper samples were prepared by High Pressure Torsion, a technique to induce high shear stresses on a specimen to produce fine grained, bulk material. The characterization of the microstructure in terms of grain size distributions, misorientation of grain boundaries and texture was done by electron backscatter diffraction. A miniaturized device for creep measurements was constructed to perform tensile creep tests under uniaxial conditions at temperatures from 273K to 348K. The measurement of the activation energy for the rate controlling creep mechanism is set into context with grain boundary diffusion experiments.

MM 37.3 Wed 15:15 H16

Creep with Single Dislocation Resolution — •Philip Egberts[1,2] and Roland Bennewitz[1,2] — [1]INM-Leibniz Institut für Neue Materialien, Campus D2 2, 66111 Saarbrücken, Germany — [2]Department of Physics, McGill University, 3600 rue University, Montreal, Quebec, H3A 2T8, Canada

Creep in materials is a result of four contributing factors: dislocation glide, dislocation creep, diffusion processes, and grain boundary climbing. Atomic Force Microscopy (AFM) is able to deform materials and detect dislocation nucleation on the atomic scale. The application of AFM to the study of creep highlights one single factor, dislocation glide. The sharp tip of an AFM probe, having a tip radius of <10 nm, was used to both image and indent KBr(100) surfaces in ultrahigh vacuum. The small tip radius and high resolution capabilities of AFM allowed for the probing of a dislocation and defect free volume while allowing for the application of stresses in the GPa range with the application of nanoNewton forces. Rapid measurements of the cantilever deflection during creep studies allow for discrete atomic pop-in events to be observed as a function of holding time. Dislocation generation for up to four minutes after reaching the maximum load is observed.

MM 37.4 Wed 15:30 H16

In-situ tensile testing of Au nanowires — •Burkhard Roos[1], Gunther Richter[2], Andreas Sedlmayr[3], Reiner Mönig[3], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Max-Planck-Institut für Metallforschung, Stuttgart — [3]Institut für Materialforschung, Karlsruhe Institute of Technology

The increase in strength with decreasing size is a ubiquitous phenomenon in metals. Particularly for free standing samples with dimensions below 100 nm, where dislocation storage is hard to envision, a convincing explanation for the size-dependent strength is missing. The goal of this study is to directly observe dislocations in small volumes, using in-situ TEM during deformation. Single crystal Au nanowires with diameters between 40 and 70 nm have been used. During deformation, crystallographic planar defects appear in the wires, remain fixed as the wire is further deformed, and then may eventually disappear. The defects nucleate homogeneously along the wire length and appear and disappear between camera frames, in less than 50 ms. In-situ tensile testing of the wires in an SEM reveals stresses at failure in the range of 0.4 and 1.5 GPa for wires with diameters between 80 nm and 400 nm. The measured stress-strain response exhibits extensive plastic flow. Post-deformation TEM studies indicate that the defects are nanotwins, which may be formed by the nucleation and motion of partial dislocations. Possible explanations for the dependence of partial dislocation nucleation on wire diameter and stress will be discussed.

MM 37.5 Wed 15:45 H16

Recrystallisation of single-phase Copper alloys investigated by resistance measurements — •Alexander Kauffmann[1,2], Jens Freudenberger[1], Hansjörg Klauss[1], Tom Marr[1,2], Konstantin Nenkov[1], Vadlamani Subramanya Sarma[3], Jürgen Eckert[1,2], and Ludwig Schultz[1,2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — [3]Dept. Metallurgical and Materials Engineering, IIT Madras, Chennai 600036, India

Copper based solid solutions with different contents of solute elements (Zn, Al, Ga, Sn, Ge) were deformed at room-temperature and at liquid Nitrogen temperature. The recrystallisation behaviour of these alloys has been investigated by means of dynamic and isothermal measurements of the resistivity (ρ). Variations of ($d\rho/dT$) from ($\rho_0\,\alpha$) are interpreted in terms of changes in defect densities by recovery and recrystallisation. Deviations from a linear temperature depedence of the resistivity increase with increasing solute concentration and depend on the stacking fault energy (γ). We observe a ($1/\gamma^2$)-dependency of the deviations which are also influenced by the deformation temperature. During deformation, γ controls the possibility to store deformation energy in the form of dislocations and deformation twins. In combination with the general trend of alloying elements to shift recrystallisation to higher temperatures, the recrystallisation behaviour of single-phase copper alloys has been described qualitatively. The observed stored dislocation and twin densities interfere with solution hardening to the macroscopic strength after deformation.

MM 37.6 Wed 16:00 H16

Simulation of the in-plane plastic anisotropy of ultrafine grained aluminum sheets produced by accumulative roll bonding — •Benoit Beausir[1], Scharnweber Juliane[1], Jaschinski Jörn[2], Brokmeier Heinz-Günter[3], Oertel Carl-Georg[1], and Skrotzki Werner[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institut für Leichtbau und Kunststofftechnik, Technische Universität Dresden, D-01062 Dresden, Germany — [3]GKSS Forschungszentrum, Max-Planck-Straße, D-21494 Geesthacht, Germany

Besides grain refinement accumulative roll bonding (ARB) leads to the formation of a texture composed of rolling and shear components. The shear components produced by friction between the rolls and the sheet are found in the surface layers. During subsequent ARB cycles, due to the bonding process the surface shear texture extends into the bulk of the sheet. Eight cycles of ARB were performed on two aluminum alloys, AA1050 and AA6016. The plastic anisotropy was investigated by tensile deformation via Lankford parameter. The global texture of the sheets was measured by neutron diffraction and used as input of the viscoplastic self-consistent model to simulate the in-plane plastic anisotropy. Simulation results are compared with those from experiment and discussed with regard to texture, strain rate sensitivity, grain shape and slip system activity.

MM 38: Mechanical Properties III

Time: Wednesday 16:30–18:00 Location: H16

MM 38.1 Wed 16:30 H16

Statistical Dislocation Dynamics: Some Comments — •Markus Hütter — Polymer Physics, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland

A statistical description of dislocation dynamics is examined from the perspective of nonequilibrium thermodynamics. Particularly, the evolution of the densities of different dislocation types is embedded into a macroscopic model for elasto-viscoplasticity. By this procedure, we discuss in detail the following points.

First, the motion of mobile dislocations is studied in order to formulate a constitutive relation for the plastic strain rate tensor in macroscopic viscoplasticity, also known as the plastic distortion rate tensor. We find a rigid connection between the Peach-Koehler force and the plastic strain rate tensor in terms of a tensorial Orowan equation. The thermodynamic driving force for dislocation motion, and for plastic flow, is identified. Specifically, a clear distinction is made between dislocation interactions and forces on dislocations due to macroscopic stress fields.

Second, we examine some frequently used reaction-type equations for mobile and immobile dislocations to model the ubiquitous strain-hardening. We demonstrate that a certain class of such models is in conflict with thermodynamic principles. The origin of this conflict is identified. Particularly, the absence of the reversal processes for any of the reactions is problematic and sharply contrasts to usual chemical reactions. Possible solutions for restoring the thermodynamic admissibility are discussed.

MM 38.2 Wed 16:45 H16

Interface fracture simulation in lamellar TiAl crystals — •Pavel Leiva Ronda, Karsten Durst, Farasat Iqbal, and Mathias Göken — Institute of General Material Properties, Department of Materials Science and Engineering, University Erlangen-Nürnberg, Germany

A microscale fracture simulation has been applied to study the toughening of lamellar TiAl crystals through interface mechanisms. The crack growth at the weak gamma -TiAl/ alpha2 -TiAl and gamma -TiAl/ gamma -TiAl lamellar interfaces has been simulated by means of a finite element method using a cohesive modelling approach. The elasticity for gamma and alpha2 phases is assumed to be anisotropic while the plasticity model considers a continuum material with a proper homogenization of the two phases lamellar system. In this sense, the constitutive plastic behaviour is described by a two-dimensional plane stress Hill's model based on reported crystal plasticity calculations. Parametric studies have been performed to investigate the effect of cohesive parameters as the energy release rate and also the influence of residual stresses on the fracture behaviour. Furthermore, it has been analyzed the relationship between bulk and interface properties within the frame of the cohesive model for the TiAl lamellar crystals.

MM 38.3 Wed 17:00 H16

Finite Auxetic Deformations of Plane Tessellations — •Holger Mitschke[1], Gerd E. Schroeder-Turk[1], Vanessa Robins[2], and Klaus Mecke[1] — [1]Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7B, 91058 Erlangen — [2]Applied Maths, School of Physics, The Australian National University, 0200 ACT, Canberra, Australia

We describe a systematic approach to study finite deformations of plane periodic symmetric skeletal structures or strut frameworks, consisting of stiff rods that pivot freely at the mutual joints. These skeletal structures are deformed by imposing a strain in one of the lattice directions and determining the response in the other lattice direction. A numerical Newton-Raphson scheme is used to find the deformation pathways that maintain constant strut lengths. The deformation behaviour is quantified by finite and instantaneous (or infinitesimal) Poissons ratios ν and ν_{inst}. This analysis allows in particular the analysis of skeletal structures based on tessellations of the plane. Applied to one- or two-uniform tesselations by regular or star polygons, this analysis reveals two as yet unknown structures with auxetic mechanisms. It also shows that a number of other periodic skeletal structure become auxetic at finite strain when retaining some or all symmetries during the deformation, some with Poisson's ratios below -1. The approach can be generalized to three-dimensional skeletal structures.

MM 38.4 Wed 17:15 H16

Effective Elastic Moduli in Solids with High Density of Cracks — •Robert Spatschek[1], Clemens Gugenberger[2], and Efim Brener[2] — [1]ICAMS, Ruhr-Universität Bochum — [2]IFF, Forschungszentrum Jülich

We investigate the weakening of elastic materials through randomly distributed circles and cracks numerically and compare the results to predictions from homogenization theories. We find a good agreement for the case of randomly oriented cracks of equal length in an isotropic plane-strain medium for lower crack densities; for higher densities the material is weaker than predicted due to precursors of percolation. For a parallel alignment of cracks, where percolation does not occur, we analytically predict a power law decay of the effective elastic constants for high crack densities, and confirm this result numerically.

MM 38.5 Wed 17:30 H16

Simulation der Ermüdung von metallischen Werkstoffen durch ein granulares Modell — •Judith Fingerhuth[1], Matz Haaks[1], Gunter Schütz[2] und Karl Maier[1] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn — [2]Institut für Festkörperforschung, Forschungszentrum Jülich

Basierend auf der Idee des zellulären Automaten wird die Akkumulation offenen Volumens bei der Ermüdung eines Metalls 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, mittlere Versetzungsdichte und Konzentration offenen Volumens repräsentiert werden. Die Veretzungsdichte erhöht sich in Abhängigkeit vom Spannungszustand des Korns, die Konzentration offenen Volumens erhöht sich nach dem Modell von Essmann, Gösele und Mughrabi und durch das Schneiden von Schraubverstetzungen. Durch Kombination mit Finite-Elemente-Methoden lässt sich im Prinzip die Ermüdung einer Probe mit beliebiger Geometrie simulieren.

Die Rechenzeit zur Simulation der eigentlichen Ermüdung einer Probe mit 10.000 Körner über eine Million Zyklen auf einem einzelnen Arbeitsplatzrechner beträgt etwa eine Stunde.

MM 38.6 Wed 17:45 H16

Performance optimized phase-field simulations of grain structures under the effect of mechanical forces — •Alexander Vondrous, Michael Selzer, Britta Nestler, and Marcus Jainta — Karlsruhe University of Applied Sciences, Moltkestr. 30, 76133 Karlsruhe

An extension of the phase-field model for polycrystalline materials is presented that incorporates the effect of mechanical forces (elasticity and plasticity) on the microstructure. We derive the set of dynamical equations and show simulations of micro cracks in grain structures under the influence of elastic stresses. Isotropic, linear elastic energies according to Hooke's law are applied in the bulk phase regions to account for the stress distribution. A new approach to describe small plastic deformations in the context of the phase-field method is based on ideal plasticity models by Tresca and von Mises criterions. We compute the wave equation of the displacement vector on a staggered grid. Modern parallel and adaptive techniques improve the performance of the numerical algorithms and allow to efficiently employ high performance clusters. As a long range objective, we aim to develop a simulation environment for microstructure formations during rolling and press hardening processes in manufacturing processes of metals.

MM 39: Topical Session Photovoltaic Materials III

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

MM 39.1 Wed 14:45 H4

Influence of interface preparation on minority carrier lifetime for low bandgap tandem solar cell materials — •Nadine Szabó, B. Erol Sagol, Ulf Seidel, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Hahn-Meitner-Platz 1 14109 Berlin

III-V semiconductor compounds grown by MOVPE are implemented in todays state-of-the-art third generation multi-junction solar cells. The current record multi junction solar cell grown on germanium, having Ge, Ga(In)As and GaInP as subcells, reached a record efficiency of 41.6%. The efficiency of these multi junction solar cells could be significantly increased, if its low bandgap Ge subcell would be replaced by a more efficient tandem. For this purpose the low bandgap materials InGaAs and InGaAsP are suitable. The bandgap composition of these materials allows a better yield of the solar spectrum. Based on InGaAs/InGaAsP absorber materials we have developed a low bandgap tandem solar cell with optimized bandgaps. Results of time resolved photoluminescence (TRPL) for the IR-bandgap compounds InGaAsP (1.03 eV) / InGaAs (0.73 eV) will be presented. The lifetime of minority carriers is one of the most important properties of solar cell absorber materials. We show on the example of the low band gap tandem cell how the choice of the materials, the quality of the bulk, the optimization of the band gap energies and the preparation of the critical interfaces are essential to build a high efficiency solar cell. The quality of the bulk and the preparation of the critical interfaces are essential for the growth of the double hetero structure (DHS).

MM 39.2 Wed 15:00 H4

Sulfosalt Gradient Layers for Photovoltaic Applications — •Herbert Dittrich, Dan Topa, Andreas Stadler, Johannes Stöllinger, Astrid Pachler, and Gerhard Aigner — Christian Doppler Labor ASEC, Universität Salzburg, Hellbrunner Str. 34, 5020 Salzburg, Österreich

Sulfosalts have demonstrated to be an important compound semiconductor family including more than 260 members. They are characterized by a complex chemistry and crystal structure. In this contribution the deposition of Sn-Sb-S gradient layers and their physical properties with respect to photovoltaic applications will be presented.

Sn-Sb-S gradient layers were deposited by magnetron sputtering from inhomogeneous targets on pure glass substrates and substrates covered with a Mo electrode layer as used in CIGS technology. Chemical analysis was carried out by electron microprobe analysis and results were combined in concentration maps over the substrate area. In correlation to the chemical composition, the structural aspects of the layers were measured by X-ray powder diffraction. The absorption coefficient, optical bandgap, resistivity, conduction type and the Seebeck coefficient of the sulfosalt layers were measured and, again, correlated to the chemical composition and the crystal structure.

Results will be discussed with respect to thin film solar cell applications.

MM 39.3 Wed 15:15 H4

Real-time investigations on the formation reactions in the system Cu-Sn-S — •Roland Schurr, Astrid Hölzing, and Rainer Hock — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstraße 3, D-91058 Erlangen

The quaternary compound kesterite Cu_2ZnSnS_4 (CZTS) is a promising candidate for the production of low-cost thin film solar cells. CZTS thin film solar cells with efficiencies of up to 6.77% were produced [1].

The understanding of the recurrent formation reactions in the system Cu-Zn-Sn-S is necessary for the optimization of CZTS absorbers and the development of low-cost thin film solar cells. In a previous publication we presented the formation of CZTS thin film solar cell absorbers from co-electroplated precursors depending on the metal ratios in the as deposited films [2]. The crystallisation of CZTS is completed by the reaction of Cu_2SnS_3 and ZnS. Further reactions mainly involved are the formation of binary and ternary Cu-Sn sulfides. Due to the phase diagrams of Olekseyuk et al. [3] of the ZnS-SnS_2 and Cu_2S-ZnS systems, the system Cu_2S-SnS_2 forms Cu-Sn sulfides at low temperatures. Real-time investigations on the formation reactions in the ternary subsystems of Cu-Zn-Sn-S while annealing stacked elemental layers provide the reaction paths of the binary and ternary sulfides.

In the present work we report on results of in-situ XRD experiments on the formation mechanisms with main focus on the Cu-Sn-S system.

[1] H. Katagiri et al., Appl. Phys. Express 1 (2008) 041201
[2] R. Schurr et al., Thin Solid Films 237 (2009) 2465
[3] I.D. Olekseyuk et al., J. Alloys Compd. 368 (2004) 135

MM 39.4 Wed 15:30 H4

Neutron diffraction investigations of kesterites: cation order and disorder — •Susan Schorr[1], Michael Tovar[2], Sergej Levcenco[3], Alexander Napetrov[3], and Ernest Arushanov[3] — [1]Free University Berlin, Institute of Geological Sciences, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Germany — [3]Academy of Sciences of Moldova Republic, Institute of Applied

Physics, Chisinau, Moldova

The quaternary chalcogenides Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ have newly attracted attention as possible absorber materials in thin film solar cells.

They crystallize in the kesterite type (space group $I\bar{4}$) or stannite type structure (space group $I\bar{4}2m$), which are described as an ordered distribution of the cations on different structural sites. Cation disorder may cause site defects and hence influences the electronic properties of the material. Thus the degree of cation order/disorder plays a crucial role and was therefor in the focus of the presented investigations. A differentiation between the isoelectronic cations Cu^+ and Zn^{2+} is not possible using X-ray diffraction due to their similar scattering power. But their neutron scattering lengths are different, thus neutron diffraction opens the possibility to determine the cation distribution in these compounds. A simultaneous Rietveld analysis of neutron and X-ray powder diffraction data revealed that in dependence on the thermal history of the samples cation disorder appears. The correlation trend between cation order/disorder and the sample growth method (solid state synthesis, Bridgemann method) will be discussed.

MM 40: Topical Session Growth Kinetics I

Time: Wednesday 16:00–17:00 Location: H4

Topical Talk MM 40.1 Wed 16:00 H4

Modeling the Role of Co-deposited Impurities in Growth: What Causes the Distinctive Step Meandering and Pyramidal Mounds on Cu(001)*— •Theodore L. Einstein[1], Rajesh Sathiyanarayanan[1,2], Ajmi BH. Hamouda[1,3], and Alberto Pimpinelli[1,4] — [1]U. Maryland, College Park, USA — [2]Now at Pennsylvania State U., USA — [3]U. Monastir, Tunisia — [4]UBP-Clermont II, France, & Science Attaché, French Consulate, Houston, TX USA

Several attempts—not involving impurities—failed to account for all the distinctive features of the growth instabilities observed on Cu vicinal surfaces;[1] recent kinetic Monte Carlo studies showed that codeposition of impurities during growth could do so.[2] To identify the responsible impurity, we compute[3] nearest-neighbor binding energies (E_{NN}) and terrace diffusion barriers (E_d) for several impurity atoms on Cu(001) using VASP. Codeposition (with Cu) of mid-transition elements (Fe, Mn, W) could cause the observed instabilities; W is most likely. Based on E_{NN} and E_d, we classify the impurities into four sets.[3] Each set produces qualitatively different surface morphologies in both the step-flow and the submonolayer ($\theta \leq 0.7$ ML) regimes. In the latter, we find the variations with θ of the number of islands and their mean size, as well as their critical nucleus size from the distribution of capture-zone areas (via fits to the generalized Wigner distribution[4]).

*Support: NSF MRSEC #DMR 05-20471; computing at NCSA, UIUC

[1]N.Néel, T.Maroutian, L.Douillard, H.-J.Ernst, JPCM 15 ('03) S3227

[2]A. Hamouda *et al.*, PRB 77 (2008) 245430; JPCM 21 (2009) 084215

[3]RS, Ph.D. thesis, UMD, 2009 [4]AP & TLE, PRL 99 (2007) 226102

MM 40.2 Wed 16:30 H4

Rectangular mound formation and rotation during grazing incidence deposition of Cu/Cu(001) — •Herbert Wormeester, Raoul van Gastel, Frits Rabbering, and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands

We have studied the consequences of oblique incidence deposition for the morphology of the growth-front for a "prototypical" system Cu/Cu(001). Electron diffraction measurements and STM show that deposition at grazing incidence leads to the evolution of rectangular mounds, oriented *perpendicular* to the plane of incidence of the atom beam. At later stages, a transition towards rectangular mounds *parallel* to the plane of incidence is observed. To elucidate the mechanisms underlying the formation of anisotropic mounds and the rotation of the mounds, quantitative kMC simulations were performed, which support and predicted experimentally observed changes in mound orientation at later stages of growth. A close contact with experiment was established by using previously determined activation barriers for intra- and interlayer diffusion processes in the simulations. The latter describe accurately the observed morphologies in a wide range of temperatures (150-300 K) and coverages up to 40 ML. The simulations show that grazing incidence leads to a very rough growth front that can be characterized as Super Poisson roughening. The strongest roughening was found to occur just before the reorientation takes place. The layer distribution is also found to be markedly different from those obtained after normal incidence growth around this transition coverage.

MM 40.3 Wed 16:45 H4

Controlled Growth of Ternary Systems due to Plasma Enhanced Chemical Vapor Deposition (PECVD) Using Metalorganic Precursors — •Markus Neubert and Volker Buck — Department of Technical Physics, University of Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

Depending on the stoichimetric ratios the physical and chemical properties of ternary systems can vary considerably. These ratios can be adjusted by parameters of the deposition process.

Ternary systems of Ti_xSiC_y were deposited in a substrat temperature range from 400°C up to 800°C using a constant flux of two metalorganic precursors and different plasma powers. Analys of films was performed by Energy Dispersiv X-Ray Spectroscopy (EDX), Secondary Ion Mass Spectrometry (SIMS)and X-Ray Diffraction (XRD) with respect to stoichiometric ratios and structure of the films. Depending on both parameters variation of the stoichiometric ratio is possible. On a limited scale simutaneous modification of plasma power and substrat temperature can compensate each other.

MM 41: Topical Session Growth Kinetics II

Time: Wednesday 17:15–18:15 Location: H4

MM 41.1 Wed 17:15 H4

Photoemission Electron Microscopy of the Temperature Dependent Pre-nucleation Dynamics of Sexiphenyl Molecules Deposited on Cu (110) — A J Fleming, F P Netzer, and •M G Ramsey — Surface and Interface Physics, Karl-Franzens Universität Graz, Universitätsplatz 5, 8010 Graz, Austria

The pre-nucleation dynamics of sexiphenyl (6P) molecules deposited in-situ on Cu (110) are investigated by photoemission electron microscopy (PEEM) in ultrahigh vacuum. PEEM, in threshold mode, is used to monitor precisely in real-time a) the amount deposited, b) layer filling by 6P molecules, c) dynamic surface density redistributions during layer filling and d) critical surface density spontaneously induced meta-stable layer de-wetting. It is by studying this crucial pre-nucleation deposition period that the requirements for critical nucleation of 6P, such as substrate commensurability, can be understood. A numerical simulation of PEEM image photoemission intensity variations with time is shown to help determine pre-nucleation layer filling mechanisms for various growth temperatures. Comparison with data previously obtained from static techniques, such as STM and NEXAFS, together with dynamic data from PEEM of 6P deposited on Cu (110) 2 x 1 * O [1] enable the 6P nucleation processes to be elucidated from PEEM.

[1] A J Fleming et al, J. Phys: Condens. Matter 21 (2009) 445003

MM 41.2 Wed 17:30 H4

Sub-monolayer growth investigations of para-sexiphenyl on sputter-modified mica(001) and SiO2 — •Stefan Lorbek[1], Gregor Hlawacek[1], Thomas Potocar[2], Adolf Winkler[2], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, 8700 Leoben, Austria — [2]Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria

Although progress has been made in recent years in the understanding of fundamental growth processes in organic molecular beam epitaxy, the underlying details are still to be explored [1]. Especially, understanding of the island nucleation on the substrate during the deposition of oligomere thin films is crucial for the design of growth routes that will avoid the undesired formation of 3D structures. Here, sub-monolayers of the rod like model molecule para-sexiphenyl (6P) have been deposited onto the isotropic surfaces of SiO2 and pre-ion bombarded mica(001) under ultra-high vacuum resulting in almost upright standing molecules. The film morphology was recorded by ex-situ atomic force microscopy. For the determination of the critical island size i*, films were grown as a function of coverage, surface temperature and evaporation rate. Three different methods were applied to determine i*: (a) Rate theory [2], scaling theory [3] and (c) capture zone scaling using Voronoi tessellation [4]. Funded by FWF(Austria).

[1] G. Hlawacek,et al., Science 321, 108 (2008) [2] J.A. Venables et al., Rep. Progr. Phys.47(1984)399. [3] J.G. Amar,F. Family, Phys. Rev. Lett.74(1995)2006. [4] A. Pimpinelli,T.L. Einstein, Phys.Rev.Lett.99(2007) 226102

MM 41.3 Wed 17:45 H4

Grain growth under limited junction mobility — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Postfach 4120, 39016 Magdeburg, Germany

Recently it has been demonstrated by experimental, theoretical and molecular dynamics simulation studies that triple lines and quadruple points of a three dimensional grain network may have finite mobilities different from the adjoining grain boundaries. Hence the kinetics of grain growth at very small grain sizes can depend also on the mobility of these boundary junctions.

We model nanocrystalline grain growth in polycrystals under the assumption that the mobility of grain boundaries is limited at small grain sizes. The standard Monte Carlo Potts model is modified by assigning each grain feature - grain boundary interface, triple line and quadruple point - its own specific mobility. For initially very small grains it can be observed that a reduction of the triple junction and quadruple point mobility leads to a change of the growth kinetics of a 3D grain network from parabolic to linear and exponential growth. These changes in the growth behaviour of the mean grain size are associated with changes in the grain size distribution. Due to the larger number of small grains the size distribution is shifted to smaller relative grain sizes. Additionally, new analytic grain size distribution functions have been calculated for the junction limited growth regimes, which are in excellent agreement with the simulation results.

MM 41.4 Wed 18:00 H4

Local grain growth kinetics in Al-Mg studied by 3DXRD microscopy — •Carl E. Krill III[1], Søren Schmidt[2], and Carsten Gundlach[3] — [1]Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany — [2]Risø DTU, Roskilde, Denmark — [3]MAX-lab, Lund University, Lund, Sweden

With the recent extension of the Mullins-von Neumann relation to 3D by MacPherson and Srolovitz comes new impetus for measuring the local kinetics of grain growth in real polycrystalline specimens. Thanks to three-dimensional x-ray diffraction microscopy (3DXRD), it is now possible to map the 3D microstructure of a single-phase polycrystalline material nondestructively, which opens up an exciting new avenue for the *in situ* study of grain growth. In this contribution, we report the microstructural characterization of hundreds of contiguous grains in a polycrystalline specimen of Al-1wt.% Mg before and after an anneal at 350°C. By measuring the displacement of individual grain boundaries, we are able to assess the local kinetics of growth (and shrinkage) for a statistically significant number of grains—information that can then be compared to the predictions of analytic models for the evolution of local and statistically averaged microstructural parameters. Exploiting the volumetric nature of the grain-boundary mapping that is delivered by 3DXRD, we conduct a direct experimental test of the extent to which the Al-Mg sample microstructure evolves as predicted by a phase-field model for grain growth under the assumption of isotropic boundary mobilities and energies.

MM 42: Topical Session Multifunctional Materials III

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

Topical Talk MM 42.1 Wed 14:45 H6

Multifunctional semiconductor nanowires for photonic applications — •Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Semiconductor nanowires are of major importance within the area of nanotechnology, and are usually synthesized using the so-called vapor-liquid-solid (VLS) mechanism. They serve as both functional units and as the wires that access them; therefore, they are ideal building blocks for multifunctional nanoscale devices. Applications and prototype devices based on semiconductor nanowires have been realized in various areas: in electronics, photonics, mechanics, and sensors. I will just summarize and focus this presentation on the use of zinc oxide nanowires for photonic applications: this will include waveguiding [1], light emitting diodes [2] and lasers [3].

[1] High order waveguiding modes in ZnO nanowires - T. Voss, G.T. Svacha, E. Mazur, S. Mueller, C. Ronning, D. Konjhodzic, F. Marlow, Nano Letters 7 (2007) 3675

[2] Scalable fabrication of nanowire photonic and electronic circuits using spin-on glass - M. Zimmler, F. Capasso, D. Stichtenoth, C. Ronning, W. Yei, V. Narayanamurti, T. Voss, Nano Letters 8 (2008) 1695

[3] Laser action in nanowires: Observation of the transition from amplified spontaneous emission to laser oscillation - M. Zimmler , J. Bao , F. Capasso , S. Mueller , C. Ronning, Appl. Phys. Lett 93 (2008) 051101

Topical Talk MM 42.2 Wed 15:15 H6

Interfaces in multifunctional perovskite oxides — •Christian Jooss[1], Joerg Hoffmann[1], Jonas Norpoth[1], Malte Scherff[1], Björn-Uwe Meyer[1], Gesine Saucke[1], and Yimei Zhu[2] — [1]Institute of Materials Physics, University of Goettingen, Germany — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, USA

Perovskite oxide materials with strong electronic or electron-lattice correlations exhibit a fascinating variety of properties from ferroelectricity over colossal resistance effects to high-temperature superconductivity. In these materials, interfaces can have a tremendous effect on the local electronic properties. This can give rise to new interfacial phases and properties which are absent in the bulk. Often, the interfacial properties strongly depend on subtle details in the atomic structure such as chemical termination layers, octahedral tilting, strain and strain relaxing interfacial defects. Therefore, the study of interfaces in perovskite oxides is a challenging subject of materials science. Topics in this talk span from the resistive switching effect at metal-manganite interfaces in pulsed electric field over new types of solar cells with correlated pn-junction to manganite-cuprate interfaces with local variation in hole doping and correlation interactions. Based on atomically resolved structural and chemical analysis, particular emphasis will be put on the study of the mechanisms of charge transfer across interfaces in the strongly correlated electron and lattice system. We give insights that well-designed oxide hetero-interfaces show a huge potential for new applications in electronics and energy conversion.

MM 42.3 Wed 15:45 H6

Diffractive optics on contact lens: application of electron beam lithography on polymer material with curved structures — •Xin Jin[1], Dawit Gedamu[1], Rainer Adelung[1], Dirk Meyners[2], Eckhard Quandt[2], Matthias Kalåne[2], Kai Rossnagel[3], Lutz Kipp[3], and Frank Spors[4] — [1]Functional Nanomaterials, Institute of Materials Science, CAU Kiel, Germany — [2]Inorganic Functional Materials, Institute of Materials Science, Faculty of Engineering, CAU Kiel, Germany — [3]Electronic Structure / Synchrotron Radiation, Institute for Experimental and Applied Physics, CAU Kiel, Germany — [4]College of Optometry, Western University of Health Sciences, Ca, USA

The principle of a diffractive bifocal contact lens was first suggested in the 1980s in the treatment for presbyopia. But the products were not successful due to problems with the reduction of the contrast in the patient*s vision. However, with progress in both the fabrication method and the design of diffractive optics (e.g., photon sieves), the question about the application of diffractive optics on contact lenses can be asked again. Therefore, in this research, zone plates and photon sieves are manufactured on contact lenses using electron beam lithography (EBL). furthermore, the problems of applying EBL on polymer contact lenses employing curved surfaces are discussed.

Acknowledgement: We thank Janine Greve for skillful technical support

MM 42.4 Wed 16:00 H6

Crossing an interface: Tuneable spin polarisation by means of electric charge — Mike Hambe[1], Adrian Petraru[2], Nikolay A. Pertsev[3], Valanoor Nagarajan[1], and •Hermann Kohlstedt[2] — [1]School of Materials Science & Engineering, University of New South Wales Sydney NSW 2052, Australia — [2]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, D-24143 Kiel, Germany — [3]A. F. Ioffe Physico-Technical Institute, Russian Academy of Science, 194021, St. Petersburg, Russia

We present experimental results on entirely complex oxide La0.67Sr0.33MnO3/BiFeO3/La0.67Sr0.33MnO3 ferromagnetic-ferroelectric-ferromagnetic tunnel junctions. The junctions were deposited by Pulsed Laser Deposition in a layer-by-layer growth mode and patterned by standard thin-film processing. We show that our devices posses a traditional Tunneling Magneto Resistance (TMR) ratio ~80% below 100 K, but that by inducing ferroelectric switching via an applied electric field of about 770 kV/cm, we can modulate the anti-parallel state resistance state as well as the TMR ratio. The experiments indicate a possible tuneable orbital reconstruction at ferromagnetic-ferroelectric interfaces via the remnant charge of the ferroelectric. The results will be discussed in the framework of the predicted magnetoelectric interface effect and may lead to novel multistate memory devices.

MM 43: Materials Design I

Time: Wednesday 14:45–16:00 Location: H5

MM 43.1 Wed 14:45 H5

Prediction by means of an evolutionary algorithm and stability of boron sheet structures — •Silvia Schumann and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

There is great interest in designing new nano materials which drives theory and experiment. Similar to carbon nanotubes and graphene there are some theoretical efforts investigating boron sheets and nanotubes. So far there are no boron sheet structures found in experiment but several sheets are suggested by theory.

We present additional work in the field of predicting boron sheets as a pre-stage to boron nanotubes. Additional to analysing already known structures we used an evolutionary algorithm reproducing those structures or discovering new boron sheets. This algorithm produces a randomly chosen population of sheets which are evaluated using pseudopotentials and plane waves to compute the free energy of each boron sheet. The more stable (lowest free energy) sheets are allowed to recombine and are mutated to form the sheets of the next generation. Promising sheets were treated with conventional structure relaxation to encounter slow convergence rates of evolutionary algorithms close to minima. We further investigated the found local minima in the energy landscape with respect to their stability by phonon calculations.

MM 43.2 Wed 15:00 H5

Stability and properties of Fe/ZrO$_2$ interfaces — •Jürgen Kutzner — TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg

The stability of the Fe/ZrO$_2$ interface was investigated by means of density functional theory. In order to estimate surface energies we carried out calculations on pure phases of iron and ZrO$_2$ for several surface orientations and phases. Further, we compared total energies and mechanical properties of different possible interface structures to predict the most stable interface structure. In order to investigate the influence of chemical composition on these properties we replaced then the pure components to simulate a simplified steel and MgO stabilized ZrO$_2$.

We would like to thank the DFG for financial support within SFB 799: TRIP-Matrix-Composite.

MM 43.3 Wed 15:15 H5

Ab initio study of nano-precipitate nucleation and growth in ferritic steels — •Natalie Tillack, Tilmann Hickel, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

The hardness of metallic alloys can be substantially improved by inducing the formation of nano-precipitates having dimensions of only a few nm. To realize such structures, chemical compositions and process conditions have to be identified that lead to a spontaneous (self-organized) formation of such structures.

For the example of ferritic alloys we have therefore studied nucleation and growth of such nano-particles combining ab initio calculations and kinetic Monte Carlo simulations. As example we consider the alloy systems Fe-Ni-Mn and Fe-Cu-Si. Using density functional theory and two supercell approaches we determine in a first step formation and interaction energies of Ni, Cu, and Si atoms in an FeMn or an Fe matrix. Our calculations reveal a repulsive interaction for pairs of Ni atoms and Si atoms, whereas the Cu-Cu and the Cu-Si interaction is attractive.

The physical origin for the different behaviour has been investigated, with a particular focus on the charge distribution and relaxation effects in the considered supercells. In a second step the ab initio determined energies are used to construct the Master equation which is solved by a Monte Carlo approach. These simulations provide a very direct insight into the formation and size distribution of the nano-precipitates as function of alloy composition, temperature and the calculated energies.

MM 43.4 Wed 15:30 H5

Epitaxial Bain Path in Transition Metals — •Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Epitaxial films grown pseudomorphically on substrates provide a way to stabilise non-equilibrium structures of materials. Obviously, there always is a certain lattice misfit between substrate and film material in its bulk equlilibrium structure. In the pseudomorphic regime, this misfit can either lead to the growth of films in a strained bulk structure or even yield structures that are not stable in the bulk. Large misfits do not necessarily imply large lateral stress. Theory can help to predict e.g. geometry, stress and magnetic properties of pseusomorphically grown metal films. In this work, we considered the fcc-bcc epitaxial Bain path (see Marcus *et al.*, PRB **66**, 064111 (2002)) of $3d$, $4d$, and $5d$ transition metals, which provides a reasonable description of tetragonally distorted films on substrates. We carried out density functional calculations in the implementation of the full potential local orbital program package FPLO (*www.fplo.de*). Emphasis is put on similarities among the transition metals.

MM 43.5 Wed 15:45 H5

On the Process of Structure Formation — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, Thin Film Group, 09107 Chemnitz, Germany

While the formation of molecules is well understood the path crystalline matter gets formed is not. Liquid and amorphous systems are intermediate states. The fundamental processes causing their structural features may help us to understand the formation of long ranging crystalline order.

For elementary systems, irrespective wether they get formed from molecular or noble gases, from polyvalent elements, from elements with 3d- or even f-states at E_F, we could show, all along the Periodic Table, that structural features of the liquid state are formed under the influence of resonances between global subsystems as there are all the electrons as one, and the forming static structure as the other one. Both mutually adjust their internal parameters, causing medium-ranging spherical periodic order (SPO) in the mean around any atom.

We discuss resonances based on momentum exchange as the driving force, causing anti-bonding (non-equilibrium) as well as bonding (equilibrium) states, with a gap or pseudogap at E_F in-between, with all the conseqences on phase stability and electronic transport. We discuss the importance of the creation of entropy whenever the system transfers to the bonding state. Instead of a thermodynamical description only we apply General Dynamics, able to describe the formation of distances and angles, the indispensable ingredients of any description of structure formation.

MM 44: Materials Design II

Time: Wednesday 16:15–17:15 Location: H5

MM 44.1 Wed 16:15 H5

Design strategy for biodegradable Fe-based alloys for medical applications — •Michael Schinhammer, Anja C. Hänzi, Jörg F. Löffler, and Peter J. Uggowitzer — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland

Iron is a promising metallic element for bioabsorbable medical implants. The aim of this article is to describe a design strategy for the development of new biodegradable Fe-based alloys for temporary implant applications, in terms of both an enhanced degradation rate compared to pure iron, and suitable strength and ductility. The design strategy is based on electrochemical, microstructural and toxicological considerations. The influence of alloying elements on the electrochemical modification of the Fe matrix and the controlled formation of noble intermetallic phases is deployed. Manganese and palladium have been shown to be suitable alloying additions for this design strategy: Mn lowers the standard electrode potential, while Pd forms noble (Fe,Mn)Pd intermetallics acting as cathodic sites. We discuss the efficiency and the potential of the design approach, and evaluate the resulting characteristics of the new alloys. The newly developed Fe-Mn-Pd alloys reveal an increased degradation rate compared to pure iron. Additionally, the mechanical performance is shown to be adjustable not only by the choice of alloying elements but also by heat treatment procedures; high strength values >1400 MPa at ductility levels >10% can be achieved. Thus, the new alloys offer an attractive combination of electrochemical and mechanical characteristics considered suitable for biodegradable medical applications.

MM 44.2 Wed 16:30 H5

Superconductivity in FeSe$_{1-x}$: a simple system with ambiguities — •Amir-Abbas Haghighirad, Mariano de Souza, Ulrich Tutsch, Sebastian Köhler, Daniel Hofmann, Michael Lang, and Wolf Assmus — Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, D-60438 Frankfurt (M), Germany

Recently, superconductivity has been reported at $\sim 8.5\,\mathrm{K}$ in FeSe with the α-PbO-type structure [1]. One of the interesting aspects of superconductivity in FeSe is the enormous effect of T_c [2,3] when pressure is applied. The latter indicates an extraordinarily high sensitivity of the superconducting state to structural deformations [4,5]. However, the accurate structure and the terminology for describing the FeSe phase that exhibits superconductivity is still not well understood. Several groups, as well as ours, have undertaken the effort to refine the synthesis steps to produce better quality single-crystalline samples of FeSe, which is crucial for resolving the physical properties, such as "anomalous" resistivity, the role of the structural phase transition as well as the role of magnetism in enabling superconductivity. We have improved our methods of synthesis using ambient- and high-pressure techniques. The effect of stoichiometry on the phase purity of FeSe and its superconducting properties were investigated. We will provide an overview of the progress seen so far. [1] F.C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (08); [2] K.W. Yeh *et al.*, Europhys. Lett. **84**, 37002 (08); [3] S. Medvedev *et al.*, Nat. Mat. **8**, 576 (09); [4] S. Margadonna *et al.*, Chem. Commun. **43**, 50607 (08); [5] T.M. McQueen *et al.*, Phys. Rev. Lett. **103**, 057002 (09).

MM 44.3 Wed 16:45 H5

Mesoporous metal catalysts formed by ultrasound — •Jana Schäferhans, Nicolas Pazos Perez, and Daria Andreeva — Physikalische Chemie II, Universität Bayreuth, Deutschland

We study the ultrasound-driven formation of mesoporous metal sponges. The collapse of acoustic cavitations leads to very high temperatures and pressures on very short scales. Therefore, structures may be formed and quenched far from equilibrium. Mechanism of metal modification by ultrasound is complex and involves a variety of aspects. We propose that modification of metal particles and formation of mesoporous inner structures can be achieved due to thermal etching of metals by ultrasound stimulated high speed jets of liquid. Simultaneously, oxidation of metal surfaces by free radicals produced in water during cavitation stabilizes developed metal structures. Duration and intensity of the ultrasonication treatment is able to control the structure and morphology of metal sponges. We expect that this approach to the formation of nanoscale composite sponges is universal and opens perspective for a whole new class of catalytic materials that can be prepared in a one-step process. The developed method makes it possible to control the sponge morphology and can be used for formation of modern types of catalysts. For example, the sonication technique allows to combine the fabrication of mesoporous support and distribution of metal (Cu, Pd, Au, Pt etc.) nanoparticles in its pores into a single step.

MM 44.4 Wed 17:00 H5

Large grain systems based on experimental EBSD-data and influence of elastic forces — •Michael Selzer, Marcus Jainta, Mathias Reichardt, Andreas Unser, and Britta Nestler — Institute for Materials and Processes, Karlsruhe, Germany

Phase-field simulations are applied to investigate the evolution of large polycrystalline grain structures from the melt or using EBSD data from experiments as initial condition. We study the dependence of grain boundary anisotropy on the evolution of the grain size distributions and the effect of misorientation distributions on the growth laws in 2D and 3D. Additionally it is possible to predict the failure and strength properties of the investigated metallic alloys. To achieve this it is necessary to take in account 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. For this goal, we present a parallel, optimized multi phase field model featuring efficient modeling 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 based on experimental EBSD data.

MM 45: HV Winter

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

Invited Talk MM 45.1 Thu 9:30 H16

"Novel" Materials for Lithium Ion Batteries and "Beyond-Lithium Ion Batteries" — •Martin Winter and Stefano Passerini — Institute for Physical Chemistry, University of Münster, Corrensstrasse 28/30, D-48149 Münster, Deutschland

Is it possible to drive 1000 km with one (present technology) battery charge? The answer to this question is presently: NO. In fact, the energy need of a mid-size car (weight: 1500kg) is about 18kWh/100km. Thus, even considering the most optimistic estimation on the development of Li-Ion batteries (200Wh/kg), which would correspond to more than 33% of the theoretical specific energy calculated on the active material weight only, it is clear that the 1000km range cannot be achieved with Li-ion (the battery weight would be more than 900kg). A revolutionary rather than evolutionary approach needs to be considered to achieve the 1000km driving range. Specific capacities close or above 1000 Ah/kg are needed for both electrodes in order to get cell specific energies at or above 1000Wh/kg. Lithium metal/element chemistries (Li/S, Li/O2 etc.) are promising to provide such high capacity, however, the long-term cycling stability of lithium metal anodes has been, so far, proved only at low charge regimes. The solution to the 1000km driving range might rely on the combination of a high energy Li/Element battery with a fast dynamic Li-Ion battery. Only "new" materials are the key to reach such a hybrid system consisting out of two batteries. This will be discussed.

MM 46: Nanostructured Materials III

Time: Thursday 10:15–11:45 Location: H16

MM 46.1 Thu 10:15 H16

Dreidimensionale Morphologie von Nanopartikeln und Nanodrähten — •Christina Möller, Z.-A. Li, M. Spasova und M. Farle — Fakultät für Physik und Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen

Der Beitrag wurde abgesagt.

MM 46.2 Thu 10:30 H16

Structure, morphology and ageing of dumbbell Ag-Fe nanoparticles — •Anna Elsukova, Zi-An Li, Mehmet Acet, Marina Spasova, and Michael Farle — Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048, Duisburg, Germany

Dumbbell-shaped nanocomposites are attracting much attention recently. Multifunctional properties of such systems offer possibilities for various diagnostic and therapeutic applications in biomedicine. [1] We have prepared dumbbell Ag-Fe nanoparticles by magnetron sputtering with subsequent in-flight annealing [2]. As-prepared particles have been aged in ambient atmosphere for 5 months. Structural properties and chemical composition of as-prepared and aged particles were examined by means of analytical electron microscopy including high-resolution imaging, energy dispersive x-ray spectroscopy (EDX) and electron energy-loss spectroscopy (EELS). As-prepared nanocomposites consist of a faceted 4-nm Ag *hat* sitting on a 10-nm Fe@gamma-Fe2O3 particle of more spherical shape. Ageing leads to the changes in the particles crystallinity and morphology. The aged nanocomposite consists of a silver spherical particle that may be attached to a hollow iron oxide sphere containing one or several silver clusters inside. Supported by DFG, SFB445. [1] Chenjie Xu et al., Angew Int Ed Engl. 2008 47(1) 173-176 [2] S. Stappert et al., J. of Cryst. Growth, 252 (2003), 440

MM 46.3 Thu 10:45 H16

Adsorption and freezing of argon in mesoporous Vycor glass — •Klaus Schappert and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus E 2.6, 66123 Saarbrücken, Germany

We explore the behaviour of argon in mesoporous Vycor glass focusing on the process of freezing and the elastic properties of the adsorbate itself. For this purpose we perform ultrasonic measurements of the effective shear modulus and of the longitudinal modulus. Isothermal filling cycles at temperatures above 66 K reveal that the first few wall-layers remain liquid-like, so that freezing starts only above a threshold [1]. From these measurements we infer the elastic properties of adsorbed wall layers with the aid of an effective medium analysis. In order to understand the behaviour of the wall layers we also conduct thermal cycles of partially filled pores down to about 15 K. At higher filling fractions, the macroscopic properties of the porous sample change abruptly, an effect that we discuss in terms of capillary sublimation.

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

MM 46.4 Thu 11:00 H16

Cluster deposition on self-assembled thiol monolayers: mechanisms from simulation and experiment — •Tommi Järvi[1], Leila Costelle[2], Minna Räisänen[3], Jyrki Räisänen[2], and Vladimir Tuboltsev[2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]University of Helsinki, Helsinki, Finland — [3]University of St Andrews, St Andrews, UK

Controlled deposition of clusters on surfaces is of vital importance in many applications of nanotechnology. Recently, cluster deposition on self-assembled monolayers (SAMs) of thiols on gold has raised interest, but open questions remain as to how the clusters interact with the thiol-covered surface on the atomic level.

Whether clusters immobilize, and retain their as-synthesized size distribution and properties, depends on the bonding between the cluster and gold substrate. Experiments show, that deposition energies of ca. 0.2-0.5 eV/at result in cluster penetration through the SAM [1,2]. High energies cause cluster deformation, however, and a thorough understanding of the cluster-SAM interaction at the atomic level is required so that desired properties can be achieved.

We address these questions using a combination of experiments and molecular dynamics simulations with a recently developed interatomic potential. We elucidate the physics of cluster landing, and show how the interplay between cluster-surface binding, deposition energy, and cluster size affects the structure of the deposited particles.

[1] Lando et al., Phys. Chem. Chem. Phys. 11, 1521 (2009).

[2] Costelle et al., unpublished.

MM 46.5 Thu 11:15 H16

Experimental demonstration of hyperbolic wave vector surfaces in silver nanowire arrays — •Jörg Schilling[1] and Jyotirmayee Kanungo[2] — [1]ZIK "SiLi-nano", Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Queen's University Belfast, Belfast, UK

Arrays of metal nanowires represent uniaxial metamaterials, whose principal effective permittivities perpendicular and parallel to the wire axis have opposite sign in the infrared and visible spectral range. This property leads to a hyperbolic equi-frequency surface for the extraordinary rays in wave vector space allowing the propagation of waves with unusally large wave vectors. Here we present an experimental mapping of the hyperbolic equi-frequency surfaces of TM (p-) polarised light propagating within a silver nanowire array. To this purpose we performed angular resolved transmission measurements on a 1.7micron high alumina film containing the silver nanowire array. From the order of the observed Fabry-Perot resonances the wave vector component kz is determined, while the lateral wave vector component kx, is obtained from the angle of incidence. The resulting markings in kx-kz wave vector diagram then result in a hyperbolic equi-frequency surface for the TM polarisation. Fitting the relationship between spectral position of the Fabry-Perot peaks and angle of incidence by a simple linear equation, we furthermore determined the values of the principal permittivities for TE and TM polarisation in a wide spectral range. All experimental results agree well with simulations based on the Maxwell-Garnett effective medium theory.

MM 46.6 Thu 11:30 H16

Plasmonic Nano Structures via Electron Beam Induced Deposition — •Katja Höflich[1,2], Ulrich Gösele[2], Jörg Petschulat[3], Norik Janunts[3], Renbin Yang[2], Andreas Berger[1,2], Thomas Pertsch[3], and Silke Christiansen[1,2] — [1]IPHT Jena — [2]MPI Halle — [3]IAP, FSU Jena

A wealth of methods have been used to create plasmonic nanostructures. Many of them lack the control needed to realize nanostructures of choice. We in our group use a dual beam instrument (FEI xP Dual Beam Nova Nanolab 600) for the direct write of nanostructures by locally cracking an organo-metallic precursor gas (dimethyl-gold(III)-acetylacetonate) with the electron beam. Therewith, it is possible to fabricate high precision structures of a few tens of nanometers in diameter with various shapes on any conductive substrate. We will present needles and pillars with tip diameters down to 10 nm as well as spirals with up to 7 windings with a diameter of 150 nm. The structures that form during decomposition of the organo-metallic precursor gas contain a matrix of carbonaceous material in which metal single crystalline nanocrystals of a few nanometers in diameter are dispersed. To densify the gold content and realize pure gold nano-needles, the carbon is oxidized out of the structures which thereby largely retain their shapes, using ozone and water vapor treatment at moderate temperatures. We present optical spectra of as-written composite and ozone treated multi-crystalline gold nanostructures that are realized on indium-tin-oxide (ITO) coated glass substrates. From these nanostructure ensembles an effective permittivity is calculated.

MM 47: Topical Session Growth Kinetics III

Time: Thursday 10:15–11:30 Location: H4

Topical Talk MM 47.1 Thu 10:15 H4

Selecting a single orientation for millimeter sized graphene sheets — •Raoul van Gastel[1], Alpha T. N'Diaye[2], Dirk Wall[3], Johann Coraux[4], Carsten Busse[2], Niemma M. Buckanie[3], Frank-J. Meyer zu Heringdorf[3], Michael Horn von Hoegen[3], Thomas Michely[2], and Bene Poelsema[1] — [1]University of Twente, Enschede, The Netherlands — [2]Universität zu Köln, Köln, Germany — [3]Universität Duisburg-Essen, Duisburg, Germany — [4]Institut Néel/CNRS, Grenoble, France

We have used Low Energy Electron Microscopy (LEEM) and Photo Emission Electron Microscopy (PEEM) to study and improve the quality of graphene films grown on Ir(111) using CVD. CVD at elevated temperature already yields graphene sheets that are uniform and of monatomic thickness. Besides domains that are aligned with respect to the substrate, other rotational variants grow. Cyclic growth/etching, exploiting the faster growth and etch rates of the rotational variants, yields films that are > 99 % composed of aligned domains. Precovering the substrate with a high density of graphene nuclei prior to CVD yields pure films of aligned domains extending over millimeters. Upon cooling, branched line defects develop in the graphene films which are grown at high temperature. We demonstrate that these defects are wrinkles in the graphene layer, i.e. stripes of partially delaminated graphene that may ultimately provide anchor points for lift-off techniques. With LEEM we observe the reversible appearance and disappearance of the wrinkles and also observe strain relaxation to take place simultaneously with the formation of a wrinkle.

MM 47.2 Thu 10:45 H4

Growth, stability and decay of cluster superlattices on the Ir(111)/graphene moiré — •Timm Gerber[1], Alpha T. N'Diaye[1], Carsten Busse[1], Josef Mysliveček[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Charles University, Praha

The moiré pattern of graphene on Ir(111) is a versatile template for the growth of two-dimensional cluster superlattices through vapour phase deposition. Using a simple growth model and kinetic Monte Carlo simulations we find that Ir cluster superlattice formation at 350 K involves the mobility of Ir momomers and Ir dimers between different moiré unit cells. Ir clusters are epitaxial, with the (111) cluster plane aligned to the (111) substrate plane and the $[1\bar{1}0]$ cluster direction aligned with the $[1\bar{1}0]$ substrate direction. In dependence of the cluster size, upon heating cluster superlattices decay through two processes: (i) complete cluster coalescence through the migration of a cluster to a neighbouring occupied moiré unit cell, where the two clusters involved reshape to a new cluster within a single moiré unit cell; (ii) incomplete cluster coalescence or cluster sintering through two clusters fluctuating in position coming into contact. Though also in cluster sintering the clusters reshape, the new sintered cluster occupies two moiré unit cells. The decay of cluster superlattices is quantitatively modelled and estimates for activation energies are obtained. Surprisingly, for all growth and decay processes modelled, we obtain extremely low prefactors. Upon heating the height distribution of clusters may improve and reshaping of single clusters without coalescence or intercell motion is observed.

MM 47.3 Thu 11:00 H4

Organic semiconductor growth on Graphene studied by LEEM and μLEED — •Gregor Hlawacek[1,2], Fawad S. Khokhar[2], Raoul van Gastel[2], Bene Poelsema[2], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, 8700 Leoben, Austria — [2]MESA+ Institute for Nanotechnology, University of Twente, NL-7500AE, Enschede, The Netherlands

The organic semiconductor para-sexiphenyl (6P) was deposited at various substrate temperatures onto graphene flakes grown on Iridium (111). The dynamics of the deposition process and the crystallographic structure were observed in-situ by means of Low Energy Electron Microscopy (LEEM) and micro Low Energy Electron Diffraction (μLEED). Layer-by-layer growth of lying molecules on graphene is observed for low deposition temperatures. After formation of a low-density layer, the full first monolayer already shows a bulk like structure. An exceptionally high mobility for 6P on graphene is observed in the initial low density layer. For room temperature the growth mode changes to Stranski-Krastanov for 6P on graphene. At elevated temperatures a continuous layer of upright standing molecules on the Ir(111) surface is nucleated by the presence of the graphene flakes.

This work is supported by the FWF project S9707-N08, STW and FOM project 04PR2318.

MM 47.4 Thu 11:15 H4

Smoothening at the organic-organic heterostructure interface — •Alexander Hinderhofer[1], Stefan Kowarik[1,2], Alexander Gerlach[1], Frank Schreiber[1], and Federico Zontone[3] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA — [3]ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble, France

In situ real-time x-ray reflectivity and complementary atomic force microscopy are used to monitor crystallinity and roughness evolution during growth of thermally evaporated organic heterostructures, using perfluoropentacene (PFP) on diindenoperylene (DIP) and pentacene (PEN) on PFP. Surface smoothening during evaporation of the second material on top of the first is observed for both systems. The smoothening mechanism can be rationalized by a lowered step edge barrier, as compared to homoepitaxy, i.e. the step edge barrier for certain molecules (PFP, PEN) is very low for diffusion on a molecular crystal of a different species (DIP, PFP). In addition, we find an exceptionally well-ordered interface for PEN-on-PFP growth and PEN growth with very low roughening. A heterostructure of these materials scatters x-rays coherently over the entire thickness.

Material combinations such as those presented here may be used as model cases for organic-organic interface engineering.

MM 48: Topical Session Growth Kinetics IV

Time: Thursday 11:45–13:00 Location: H4

Topical Talk MM 48.1 Thu 11:45 H4

X-radiographic video microscopy studies of alloy solidification processes — •Ragnvald H Mathiesen[1] and Lars Arnberg[2] — [1]Department of Physics, NTNU, N-7491 Trondheim, Norway — [2]Department of Materials Technology, NTNU, N-7491 Trondheim, Norway

The combination of state-of-the art synchrotron X-ray sources and recent developments in X-ray hardware such as focusing optics and fast low-noise high-resolution cameras have opened for in situ studies of solidification processes at spatiotemporal resolutions approaching and even beyond those that can be achieved with optical video microscopy. An overview of recent case studies with Al-Cu and Al-Si based binary and tertiary systems will be given, with particular focus on how the experimental results compares qualitatively and quantitatively with results from modeling at the length and time scales of diffusive and convective mass transport. Finally, results from recent experiments will be presented showing how the boundaries of radiographic performance can be extended both spatially and temporally to address faster dynamics and approach capillarity limited kinetics.

MM 48.2 Thu 12:15 H4

Anomalous dendrite growth in undercooled melts of Al-Ni alloys — Roman Lengsdorf[1,2], •Dirk Holland-Moritz[1], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

We have measured dendrite growth velocities as a function of undercooling on liquid Al-Ni alloys using electromagnetic levitation on Earth and in reduced gravity. In total, six differently concentrated alloys are investigated, one of them for comparative investigations during the sounding rocket mission TEXUS 44. While on the Ni-rich side of Al-Ni alloys growth velocity is increasing with increasing undercooling, Al-rich Al-Ni alloys show an unusual decrease of the growth velocity with increasing undercooling in the terrestrial investigations. The comparison of the results of complementary terrestrial and microgravity experiments suggests that the anomalous growth behavior of Al-rich Al*Ni alloys may be caused by fluid-flow related processes during non-equilibrium solidification of undercooled melts. Support by ESA within contract number 15236/02/NL/SH (NEQUISOL) and by the European Commission EC under contract FP6-500635-2 (IMPRESS) is gratefully acknowledged.

MM 48.3 Thu 12:30 H4

Undercooling and solidification of Ni_2B under different convective flow conditions — •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 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 a suitable 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 HE1601/25.

MM 48.4 Thu 12:45 H4

In Situ Observation of Dislocation Dynamics at the TOPO-TOMO Beamline at the Synchrotron Light Source ANKA — •Andreas Danilewsky[1], Jochen Wittge[1], Arne Cröll[1], Adam Hess[1], David Allen[2], Patrik McNally[2], Patrick Vagovic[3], Zhijuan Li[3], Tilo Baumbach[3], Eider GorosteguiColinas[4], Jorge Garagorri[4], Reyes Elizalde[4], Matteo Fossati[5], Keith Bowen[5], and Brian Tanner[5] — [1]Kristallographie, Universität Freiburg — [2]RINCE, Dublin City University, Ireland — [3]ANKA, ISS, Research Center Karlsruhe — [4]CIT, Sab Sebastian, Spain — [5]Physics Dept., Durham, UK

White beam X-ray topography at the Topo-Tomo beamline of the synchrotron light source ANKA (Research Centre Karlsruhe) is used to monitor in situ the origin and the dynamics of dislocations in silicon at high temperatures. The (100) Si sample with well defined, artificial defects from a nanoindenter was heated in a mirror heater up to 1000°C. During the heating the transmission X-ray topographs were taken with a CCD-camera system continuously every second resulting in a movie of the formation and motion of dislocations. It will be shown, that the indents act as the source for dislocation loops. The dislocations move with about 3.4 x 10-5 m/sec inside two opposite inclined {111} glide planes. Finally slip bands of 60°-dislocations are formed. The experimental details of the high temperature topography, the analysis of dislocations as well as the first results of the dislocation dynamics and slip band formation will be presented.

MM 49: Topical Session Battery Materials I

Time: Thursday 10:15–11:45 Location: H6

Topical Talk MM 49.1 Thu 10:15 H6

Mechanisms of intercalation, ionic motion and new metastable cathode materials — •Stanley Whittingham — SUNY, Binghamton, NY, USA

Intercalation is the predominant reaction mechanism in rechargeable batteries in use today. Intercalation processes, unlike conversion reactions, allow for fast ionic motion both on lithium insertion and lithium removal. Moreover the structural maintenance during reaction permits essentially unlimited cycling of the material.

Intercalation can occur within a single phase as originally demonstrated in titanium disulfide, or with the formation of a second phase, as demonstrated in vanadium diselenide, the manganese oxide spinels and most recently in the lithium iron phosphate olivine. Although two-phase reactions were thought to be rate-limiting, such is not necessarily the case.

Ionic motion will be compared in materials with different intercalation mechanisms, and for thermodynamically stable as well as metastable compounds. This work is being supported by the United States Department of Energy, Energy Frontier Research Center.

Topical Talk MM 49.2 Thu 10:45 H6

Ion conductivity and effects of mechanical treatment — •Paul Heitjans and Martin Wilkening — Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, D-30167 Hannover

A way to enhance the ionic conductivity of materials being suitable, e.g., for batteries is to reduce the crystallite size. The largely increased volume fraction of interfacial regions in nanocrystalline ceramics provides pathways for fast cation as well as anion diffusion. Nanostructuring can easily be achieved by high-energy ball milling. We will review studies on single- and two-phase ion conductors such as $Li_4Ti_5O_{12}$, $LiTaO_3$, $LiNbO_3$ and Li_2O:Al_2O_3, BaF_2:CaF_2, respectively, serving as model substances to investigate the effect of mechanical treatment on the ionic diffusivity. As an example, ball milled nanocrystalline $LiTaO_3$ - even when treated in a shaker mill for only 30 min - exhibits an increase of the overall room temperature Li conductivity by about five orders of magnitude compared to that of the coarse grained source material. Mechanical treatment of BaF_2 and CaF_2 together for about 32 h in a shaker mill leads to a composite material where the anion conductivity is increased by a factor of 10^3 compared to that of single-phase nanocrystalline BaF_2 prepared under the same conditions. Besides conductivity measurements we used a variety of ^7Li and ^{19}F solid state NMR techniques to gain detailed information about the dynamics as well as first insights into the microstructure of these highly defective materials.

MM 49.3 Thu 11:15 H6

Determination of the lithium diffusion coefficient in novel anode materials based on graphite/SiCN composites — •Andrzej P. Nowak, Magdalena Graczyk-Zajac, Claudia Fasel, and Ralf Riedel — Institute of Materials Science, Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

Commercially available anode materials for lithium ion secondary batteries are based on graphite due to its cycle stability, low price, easy to handle and reversible capacity of 372 mAh/g. This type of anode material is suitable for high energy application. However, there is still a need for new materials for high power applications. Here, we report on novel graphite/SiCN composite materials which exhibit promising electrochemical performances for high energy and high power density batteries. For high energy application the ratio graphite to preceramic polymer is 3:1 and the capacity reaches a value of 600 mAh/g. For high power application the starting materials ratio is 1:1 and the capacity after 200 cycles has been determined to be about 200 mAh/g. The correlation between electrode capacity and the graphite/SiCN ratio, the pyrolysis temperature and materials composition has been established. The relation between these parameters as well as the lithium diffusion coefficient in the novel electrode materials was calculated from the results obtained from EIS, CV and GITT studies. The direct dependence between the lithium diffusion coefficient and the materials electrochemical properties is discussed.

MM 49.4 Thu 11:30 H6

Atom probe tomography of solid state ion-conductive mem-

branes — •Gerd-Hendrik Greiwe, Guido Schmitz, and Frank Berkemeier — Institut für Materialphysik WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Deutschland

Our group has long-termed interest in glassy ion-conductive membranes to be used in all solid state batteries. Using ion beam sputtering methods, we could demonstrate that thin film membranes of amorphous Li-borate glass reveal a conductivity even better than quenched bulk glasses and furthermore a finite-size effect was documented (1,2). However, the Li content of sputter deposited thin films could not be determined by conventional EDX or EELS analysis due to the low mass of Li.

In new experiments, we measure the Li content of the glass by means of laser-assisted atom probe tomography. For this, glass layers and suitable electrodes are deposited upon pre-shaped tungsten tips. Although quite complex, the obtained mass spectra are well understood in terms of various molecular species so that a quantitative analysis gets possible. It is indicated that the reported finite-size effect is due to indiffusion of Li from the electrode materials.

(1) F. Berkemeier, M.R. Abouzari, and G. Schmitz, Phys. Rev. B 76, (2007) 024205.

(2) F. Berkemeier, M.R. Abouzari, G. Schmitz, Ionics, DOI 10.1007/s11581-008-0266-4.

MM 50: Topical Session Battery Materials II

Time: Thursday 12:15–13:00 Location: H6

Topical Talk MM 50.1 Thu 12:15 H6

Hysteresis due to non-monotone material behaviour inside many particle systems — •Clemens Guhlke and Wolfgang Dreyer — Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany

Relying on two examples we study storage problems. The examples concern the storage of lithium in small iron phosphate particles constituting the cathode of a lithium-ion battery and the storage of air in elastic rubber balloons.

The two storage systems have in common: 1. The iron phosphate particles as well as the rubber balloons exhibit non-monotone constitutive behavior. 2. Phase transition and hysteresis during loading and unloading.

We describe the processes of loading and unloading by a kinetic equation of Fokker-Planck type. There are two small parameters that control whether the phase transition evolves along the Maxwell line or if they exhibit strong hysteretic behavior.

MM 50.2 Thu 12:45 H6

Thermodynamics and electronic structure of intrinsic point defects in LiCoO$_2$ — •Melanie Gröting and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, D-64342 Darmstadt

A key problem of rechargable battery devices is their degradation. Various processes including 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. Therefore a detailed understanding of these mechanisms is important for improving the materials properties. In this study we present density-functional theory calculations (DFT) of intrinsic point defects in LiCoO$_2$ using the supercell approach. Formation energies are calculated and the electronic structures and density of states are examined in order to compare them with XPS data. Also, the thermodynamic stability of Li$_x$CoO$_2$ with lithium contents x = 1.0, 0.5 and 0 is determined with respect to the competing metal oxides. We consider lithium and cobalt vacancies, as well as oxygen vacancies and interstitials. An important finding is that besides oxygen defects cobalt vacancies can dominate under certain conditions.

MM 51: Electronic Properties I

Time: Thursday 10:15–11:15 Location: H5

MM 51.1 Thu 10:15 H5

Momentum resolved Eliashberg function calculations within the KKR formalism — •Sergiy Mankovsky, Jan Minar, and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, Universität München, Butenandtstr. 11, D-81377, München, Germany

We present an expression for the calculation of the momentum resolved Eliaschberg function $\alpha^2F(\omega,\vec{k})$ within the KKR Green's function formalism. All underlying calculations of the electron-phonon matrix elements as well as of the phonon energies are based on ab-initio electronic structure calculations performed using the fully relativistic spin-polarised KKR band structure method. Applications have been done for various non-magnetic as well as for magnetic systems. The Eliaschberg function obtained within these calculations have been used to evaluate the electron-phonon self-energy $\Sigma_{\vec{k}}$. The self-energies obtained are compared with those obtained from angle resolved photoemission spectroscopy (ARPES). In all cases studied so far a very satisfying agreement was achieved.

MM 51.2 Thu 10:30 H5

First-principles electronic structure and chemical bonding studies of type I clathrates Ba$_8T_xE_{46-x}$ (T: late transition metals; E: Si, Ge; x = 0–6) — •Alim Ormeci, Umut Aydemir, Wilder Carrillo-Cabrera, Michael Baitinger, and Yuri Grin — Max Planck Institute for Chemical Physics of Solids, Dresden

In recent years type I clathrates doped with transition metals have attracted a lot interest largely due to the expectations that such materials may have interesting electronic and transport properties. The cubic unit cell of type I clathrates contains two 20- and six 24-framework atom cages. The voids enclosed by these cages can be filled with alkali, alkaline-earth or rare earth metals, while transition metals or Ga can substitute some of the framework atoms yielding three-component compounds. Here, the interest is confined to Si or Ge as main framework atoms, Ba as filler, and some late transition metals selected from Groups 9-12 as dopants. The dopants usually occupy the 6*c* Wyckoff position (space group $Pm\bar{3}n$, no. 223), however the range of 6*c* site occupation fraction depends on the dopant and the framework atom, Si or Ge. Vacancies at 6*c* sites are a possibility and observed mostly in Ge clathrates rather than in Si ones. Using the full-potential local orbital (FPLO) method and supercells containing up to 216 atoms, electronic structures, chemical bonding and heats of formation will be investigated for the systems Ba$_8T_xE_{46-x}$ with E: Si, Ge and for x = 0–6 allowing also for the possibility of vacancies, as well. Theoretical results will be compared with experimental findings.

MM 51.3 Thu 10:45 H5

Optical and electrical characterization of Al doped Zinc oxide nanoporous films prepared via sol-gel method — •Babak Nasr, Subho Dasgupta, Robert Kruk, and Horst Hahn — Karlsruhe Institute of Technology (KIT) GmbH,Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Highly transparent and conducting ZnO films doped with different Al concentration prepared via sol-gel method. In this study one of the most important deposition parameters, heat ramping at pre-heat-treatment step, was investigated to grow high porous thin films in high surface area applications. It was found that high porosity is obtainable by fast heat ramping of the gel films. In addition the optical and electrical properties of Al doped ZnO films as a function of carrier concentration was studied using UV-Vis, FTIR spectroscopy, and four points measurement. The films were all transparent in visible range and had a sharp absorption around 380 nm. A blue shifts of the absorption edge respect to undoped ZnO has been observed as a function of the carrier concentration up to 2 at.% Al doping due to Burstein-Moss effect. Strongly resonance absorption at plasma frequency in near infra red region led to calculation of carrier concentration. These investigations were complemented by photoconductivity measurement to understand the impact of surface states in electronic structure of the films. Among different doped films with atomic ratio of 0.5 to 4 with increments of 0.5 the systems with 1.5at.% to 2at.% show the lowest resistivity and widest optical band gap.

MM 51.4 Thu 11:00 H5

Positronic structure in metals containing vacancies — •Martin Offenberger[1], Hubert Ebert[1], and John Banhart[2] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz Zentrum Berlin

Positron anihilation is a well established tool to study defects in metals. Corresponding theoretical calculations for the positronic structure for such systems are made so far using standard band structure codes together with the so-called super cell approach. We present a fully relativistic approach that makes use of multipe scattering theory, i.e. the Korringa-Kohn-Rostoker Green's function (KKR-GF) method, to avoid artificial boundary conditions. This is achieved by dealing with the defect region by means of the Dyson equation. First results will be presented for the density of states and charge distributions for a positron captured by a vacancy in various metals as Al, Cu and Fe. The change of these properties due to adjacent impurities will be discussed in addition.

MM 52: Electronic Properties II

Time: Thursday 11:30–13:00 Location: H5

MM 52.1 Thu 11:30 H5

***Ab initio* investigation of the Spin Hall Effect for non-magnetic alloys** — •Stephan Lowitzer, Diemo Ködderitzsch, and Hubert Ebert — Department Chemie, Physikalische Chemie, Universität München, Butenandstr. 5-13, 81377 München, Germany

Spin-orbit coupling is responsible for several interesting phenomena like e.g. the anomalous Hall effect (AHE) in magnetic materials. The AHE results from the interaction between spin-orbit coupling and the spin polarization. In comparison to the AHE the spin Hall effect (SHE) needs no spin polarization and is therefore even present in non-magnetic systems. This was shown by several experimental works e.g. [1].

During the last years several publications have appeared which studied the spin Hall effect for pure systems via *ab initio* e.g. [2] or model calculations [3]. However, up to now no publication is available in which the SHE is calculated for alloy systems on an *ab initio* level.

To calculate the SHE we have implemented the Kubo-Středa equation in our fully relativistic SPR-KKR package. The Kubo-Středa equation gives access to the full anti-symmetric conductivity tensor what is necessary for the calculation of the SHE. The disorder is treated via the coherent potential approximation (CPA). We show first results for several non-magnetic $3d$ and $4d$ transition metal alloys.

[1] S. O. Valenzuela and M. Tinkham, Nature **442**, 176 (2006)
[2] Y. Yao and Z. Fang, Phys. Rev. Lett. **95**, 156601 (2005)
[3] T. Tanaka, M. Kontani, M. Naito, T. Naito, D. S. Hirashima, K. Yamada and J. Inoue, Phys. Rev. B **77**, 165117 (2008)

MM 52.2 Thu 11:45 H5

FeSe$_{1-x}$ synthesized under ambient- and high-pressure conditions: a comparative study — •Mariano de Souza, Amir-Abbas Haghighirad, Ulrich Tutsch, Sebastian Köhler, Daniel Hofmann, Michael Lang, and Wolf Assmus — Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, D-60438 Frankfurt (M), Germany

Among the Fe-based superconducting (SC) materials, the binary alloy FeSe$_{1-x}$ with $T_c \simeq 8.5\,\mathrm{K}$ [1] has attracted enormous interest. Although a tetragonal-to-orthorhombic transition at high-T takes place, it is not accompanied by long-range magnetic ordering, as it occurs in other Fe-based superconductors. Many questions remain still open, like the right stoichiometry of the SC phase, the symmetry of the SC order parameter and the origin of the high-pressure dependence of T_c [2]. Here, we report resistivity, susceptibility and thermal expansion data on single-crystalline FeSe$_{0.95}$ prepared under ambient- and high-pressure (HP) conditions. We show that SC samples of FeSe$_{1-x}$ can also be obtained well outside the composition range reported in the literature [3]. Our thermal expansion results reveal a tiny feature around ~90 K, most likely related to the structural phase transition, and onset of superconductivity around 8.5 K. For samples synthesized under HP conditions, the saturated magnetic moment of Fe is dramatically reduced and superconductivity is destroyed. [1] F.-C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 1462 (08); [2] S. Medvedev *et al.*, Nat. Mat. **8**, 576 (09); [3] T.M. McQueen *et al.*, Phys. Rev. B **79**, 014522 (08).

MM 52.3 Thu 12:00 H5

Groundstatable fermionic wavefunctions and their associated many-body Hamiltonians — Daniel Charrier[1] and •Claudio Chamon[2] — [1]Max Planck Institut für Physikkomplexer Systeme, Nöthnitzer Straße38, 01187 Dresden, Germany — [2]Physics Department, Boston University, Boston, MA 02215, USA

In the vast majority of many-body problems, it is the kinetic energy part of the Hamiltonian that is best known microscopically, and it is the detailed form of the interactions between the particles, the potential energy term, that is harder to determine from first principles. An example is the case of high temperature superconductors: while a tight-binding model captures the kinetic term, it is not clear that there is superconductivity with only an onsite repulsion and, thus, that the problem is accurately described by the Hubbard model alone. Here we pose the question of whether, once the kinetic energy is fixed, a candidate ground state is groundstatable or not. The easiness to answer this question is strongly related to the presence or the absence of a sign problem in the system. When groundstatability is satisfied, it is simple to obtain the potential energy that will lead to such a ground state. As a concrete case study, we apply these ideas to different fermionic wavefunctions with superconductive or spin-density wave correlations.

MM 52.4 Thu 12:15 H5

Ab initio electron correlation calculations for the structural properties of Cadmium — •Beate Paulus[1], Nicola Gaston[2], Dirk Andrae[1], Ulrich Wedig[3], and Martin Jansen[3] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin — [2]Industrial Research Limited, Gracefield Research Centre, PO Box 31-310, Lower Hutt, New Zealand — [3]Max Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

Cadmium crystallises in the hcp structure, but with an anomalously large c/a ratio, indicating a strong distortion away from ideal packing. Coupled cluster calculations within the framework of the method of increments with an embedding scheme for metals were performed to explore the potential energy surface of cadmium with respect to the hexagonal lattice parameters [1]. This potential energy surface is compared to density functional theory based surfaces, as calculated with various functionals. The overall behaviour of the method of increments for cadmium is consistent with previous results for zinc [2], emphasising the dominant role of electronic correlation in achieving a sufficiently accurate description of bonding properties for the two elements; however, a detailed analysis shows differences.

(1) N. Gaston, D. Andrae, B. Paulus, U. Wedig, and M. Jansen, Phys. Chem. Chem. Phys., 2010, DOI: 10.1039/b915967c

[2] N. Gaston, B. Paulus, U. Wedig, and M. Jansen, Phys. Rev. Lett. 100, 226404 (2008).

MM 52.5 Thu 12:30 H5

Efficient and accurate method for calculating properties of random alloys with short-range order — •Oleg Peil[1], Andrei Ruban[2], and Börje Johansson[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Department of Materials Science, Royal Institute of Technology, Sweden

We present an efficient and accurate method for calculating properties of alloys with short-range order. The method is based on the Green's function approach in the framework of the exact muffin-tin orbital (EMTO) [1] fomralism. An alloy system is represented by a supercell with short-range order parameters controlled up to high coordination sphere numbers (4-10), and the local Green's function of each atom is calculated exactly within the local interaction zone (LIZ). The key ingredients of the method are locality, which makes it linearly-scaling with the number of atoms in the supercell, and self-consistency of the effective medium, which results in fast convergence of the total energy and density of states with respect to the LIZ size.

To test the performance and accuracy of the developed method, we show by several examples that for ordered alloys it correctly reproduces the density of states and total energy for both the single-site limit (LIZ=1) and ordered limit (LIZ→ ∞). The method is then applied to two systems: Fe_2Si and Fe-rich bcc-FeCr that have a strong dependence of the local magnetic moments and interatomic interactions on the local environment.

[1] L. Vitos, Phys. Rev. B **64**, 014107 (2001)

MM 52.6 Thu 12:45 H5

Fermi surface shrinking and interband coupling in iron-based pnictides — •Luciano Ortenzi[1], Emmanuele Cappelluti[2], Lara Benfatto[4,3,2], and Luciano Pietronero[3,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]SMC Research Center, CNR-INFM, c/o ISC-CNR, via dei Taurini 19, 00185 Rome, Italy — [3]Dipart. di Fisica, Università “La Sapienza”, P.le A. Moro 2, 00185 Rome, Italy — [4]Centro Studi e Ricerche “Enrico Fermi”, v. Panisperna 89/A, 00184, Rome, Italy

Measurements of Fermi surface with de Haas-van Alphen oscillations in LaFePO showed a shrinking of the Fermi pockets with respect to first-principle LDA calculations, suggesting an energy shift of the hole and electrons bands with respect to LDA. In this talk I will show that these shifts are a natural consequence of the strong particle-hole asymmetry of electronic bands in pnictides, and that they provide an indirect experimental evidence of a dominant interband scattering in these systems. Recent measurement in 122 systems confirm this picture.

MM 53: Nanostructured Materials IV

Time: Thursday 14:00–15:00 Location: H16

MM 53.1 Thu 14:00 H16

Strain in the nanograin — •Harald Rösner and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

Strain in an individual deformation-twinned nanocrystalline Pd grain of about 24 nm size was mapped. The in-plane components of the strain tensor were calculated and charted using geometric phase analysis based on an individual high-resolution transmission electron microscopy image. Considerable shear strain was accumulated along the twin boundaries. The twins and matrix were significantly distorted relative to each other (rotated by about 3° on average) and showed a strong gradient across the grain running parallel to the twin lamellae. An estimate of the strain energy stored in the Pd grain yielded a value of E = 6.495 J/g. Based on the strain distribution observed, a temporal deformation scenario is discussed.

MM 53.2 Thu 14:15 H16

Melting behaviour of embedded Pb nanoparticles in an Al (Ga) matrix — •Anna Moros, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Melting is one of the most important phase transformation in nature, but its underlying mechanism is still not completely understood. It is well known, that decreasing particle sizes lead to a change of the bulk properties of a material, as for instance a shift of the melting point. Current investigations on the melting behaviour of Pb nanoparticles embedded in an Al matrix are presented. In contrary to the prediction of many models for size-dependent melting, faceted and truncated cuboctahedric Pb nanoparticles with a cube-on-cube orientation relationship to the matrix start to melt 10 - 30 K above the melting point of the bulk material, indicating a more complex dependence of the melting temperature with respect to the particle-matrix interfaces. Here, the melting temperature of the particles was determined by means of differential scanning calorimetry. The size distribution of Pb inclusions in the samples was obtained from TEM images. However, it was observed that the addition of Gallium selectively into the Al matrix led to a significant shift of the melting temperature of the Pb nanoparticles. The experimental results are presented and discussed.

MM 53.3 Thu 14:30 H16

Finite Size Effects in Oxide Nanoparticles — •Manuel Diehm, Peter Agoston, and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt

Nanoparticles of several oxide materials with different structures and morphologies are investigated by molecular statics simulations in order to study the implications of finite size effects. Interatomic interaction was described by Coulomb/Buckingham pair-potentials and special attention was given to the role of missing long-ranged Coulomb interactions and related structural relaxations. It is discussed under what conditions volume and surface contributions to the lattice energy of ionic nanoparticles become extensive quantities. Further, it is examined how the presence of point defects affects the lattice energy and the range of resulting disturbances in the ideal Coulomb potential at surrounding lattice sites.

MM 53.4 Thu 14:45 H16

Simulation of the gyroid phase in copolymer systems — •Alexei Karatchentsev[1], Wolfgang Dieterich[2], Philipp Maass[3], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

We employ a coarse-grained model to study the formation of periodic continuous mesostructures in diblock and triblock copolymer melts. Within this model, the blocks of the copolymer molecule are mapped onto soft spheres with fluctuating radii of gyration and the distance between the centers of the spheres [1]. The probability distribution functions for these quantities as well as the monomer number densities of the blocks are derived from the Gaussian chain model. The kinetics of the mesophase segregation is driven by a Monte-Carlo algorithm. First we explore in detail the gyroid phase observed in the diblock copolymer system and discuss its stability. Then we study the system of linear triblock copolymers and show how such system can possibly increase the region of stability of the gyroid phase.

[1] F. Eurich, A. Karatchentsev, J. Baschnagel, W. Dieterich, and P. Maass J. Chem. Phys. 127, 134905 (2007)

MM 54: Nanostructured Materials V

Time: Thursday 15:15–17:00 Location: H16

MM 54.1 Thu 15:15 H16

Understanding the growth mechanism of carbon nanotubes via the "cluster volume to surface area" model — •Sreekanth Mandati[1,2], Jens Kunstmann[1], Felix Börrnert[3], Ronny Schönfelder[3], Mark Rümmeli[3], Kamal K. Karb[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [2]Indian Institute of Technology, Kanpur, India — [3]Institute for Solid State Research, IFW Dresden, Germany

The influence of mixed catalysts for the high yield production of carbon nanotubes (CNTs) has been studied systematically. Based on extensive experimental data a "Catalyst Volume to Surface Area" (CVSA) model was developed to understand the influence of the process parameters on the yield and CNT diameter distribution [1]. In our study, we present a refined version of the CVSA model developed by combining experiments and simulations. We discuss our current understanding of the growth mechanism and how the model might be used to increase CNT yields by using mixed catalysts. [1] S. Tetali et al., ACS Nano (2009), DOI: 10.1021/nn9012548.

MM 54.2 Thu 15:30 H16

Controlling the kink angle of intramolecular carbon nanotube junctions: A combined experimental and theoretical study — Jan Blüher[1], •Jens Kunstmann[1], Imad Ibrahim[1], Alicja Bachmatiuk[2], Felix Börrnert[2], Mark Rümmeli[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [2]Institute for Solid State Research, IFW Dresden, Germany

Intramolecular carbon nanotube (CNT) junctions are nanotubes with kinks generated by heptagon-pentagon defect pairs. They are very attractive functional building blocks for future electronics, as they can be used as diodes and transistors. Usually CNT junctions are synthesized incidentally [1]. Using chemical vapor deposition techniques we are trying to grow CNT junctions in a more controlled way. In particular, we want to control the kink angle in order to produce junctions with well defined electronic properties. Our approach raises the question: Are there special kink angles that induce a certain change in electronic properties? In order to answer this question we developed a scheme that allows generating the atomic structure of CNT junctions with an arbitrary number of heptagon-pentagon defects. To break down the large number of different geometrical possibilities to achieve a CNT junction with a specific angle we study the energetics of different defect combinations and discuss the implication of these results for the experimental realization of well defined CNT junctions. [1]Wei et al., Adv. Mater. 20, 2815 (2008).

MM 54.3 Thu 15:45 H16

Direct imaging and analysis of the internal interfaces between carbon nanotubes and their catalyst particles — •Darius Pohl[1], Franziska Schäffel[1], Christine Täschner[2], Mark Hermann Rümmeli[2], Christian Kisielowski[3], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, IMW, Dresden, D-01171, Germany — [2]IFW Dresden, IFF, Dresden, D-01171, Germany — [3]NCEM, LBNL, Berkeley, CA 94720, USA

The functionalization of the ends of the CNT has become an important research field due to the potential to hereby modify their physical properties. Functionalized CNT can thus be used to build up new micro-scaled structures with high performance. Owing to its large magneto-crystalline anisotropy energy, L10 ordered FePt is among the most intensively discussed materials when it comes to pushing the superparamagnetic limit towards minimum particle sizes. As a consequence, this material is of particular interest for the realisation of a hard-magnetic termination of the CNT. CNTs as obtained grown via PE-CVD from Fe-Pt multi-layer thin films are characterized by means of aberration-corrected HRTEM. In order to gain a deeper insight into the growth mechanism structural investigations are focused on the atomically resolved characterisation of the FePt-CNT interface. First results on the atomic structure of this metal-carbon interface will be presented. Near-interface lattice expansion is observed which is attributed to Pt segregation towards the surface of the catalyst particle. The results of the structural characterization will be compared with the thermodynamically favoured nucleation sites of the graphitic layers.

MM 54.4 Thu 16:00 H16

Magnetomechanical Interactions in Freestanding, Ferromagnetically Filled Carbon Nanotubes — •Stefan Philippi, Uhland Weissker, Markus Löffler, Thomas Mühl, Albrecht Leonhardt, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany

The extraordinary mechanical properties of carbon nanotubes (CNT) yield enormous potential for applications in nano-electromechanical systems (NEMS). Yet almost all of the proposed or already implemented NEMS are actuated via electrical effects. Employing CNT with ferromagnetic filling will offer alternative applications for magnetically driven NEMS, if both their magnetic and mechanical properties are equally well understood. In this talk, several static and dynamic effects of applied magnetic fields on filled CNT are discussed with regard to fundamental analyses of their magnetomechanical properties as well as basic principals for potential applications.

MM 54.5 Thu 16:15 H16

Synthesis and mechanical properties of iron-filled carbon nanotubes — •Uhland Weissker, Markus Löffler, Franziska Wolny, Thomas Mühl, Albrecht Leonhardt, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Deutschland

Iron-filled carbon nanotubes (CNTs) are a promising material for magnetic applications. In addition to their interesting magnetic properties their mechanical properties are also very important for applications as probes for magnetic force microscopy (MFM) or actuators.

The mechanical properties of iron-filled multi-walled carbon nanotubes were investigated by static and dynamic bending methods.

It was found that a modified Euler-Bernoulli beam model, accounting for the mounting of the CNT on a substrate and characteristic structural defects, can be used to evaluate and explain the experimental data in order to obtain the mechanical properties. Dominating defects influence the mechanical behavior which is expressed by an eigen mode frequency ratio that differs from that of an ideal beam. Furthermore, the shape of the envelope of the resonant vibration state is evaluated.

It is also shown that the resonance frequency of the CNTs can be tailored by etching the CNTs in a water vapor environment inside a scanning electron microscope (SEM). The mechanical properties of iron-filled CNTs are comparable to that of unfilled multi-walled CNTs, thus they are promising material for MFM probes.

MM 54.6 Thu 16:30 H16

Current-induced shaping of carbon nanotubes and their filling — •Markus Löffler, Stefan Philippi, Uhland Weissker, Thomas Mühl, Thomas Gemming, Rüdiger Klingeler, and Bernd Büchner — IFW Dresden, (P.O. box 270116, 01171 Dresden,) Germany

With the help of an in-situ nanomanipulator, structural changes and mass transport phenomena in filled and empty multi-wall carbon nanotubes (MWCNT) under electrical bias have been studied inside a transmission electron microscope. The inter-shell resistance has been determined by subsequently removing nanotube shells with short time high bias transport. Electromigration and thermal activation have been determined as the main causes of current-driven mass transport, which has been studied in different regimes. Especially, fully reversible mass transport inside a MWCNT as well as current-induced directed growth of carbonaceous nanostructures has been observed. The knowledge of the measured 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 54.7 Thu 16:45 H16

Photoluminescence on single-walled carbon nanotubes: A recipe to relative signal intensities — •Sebastian Heeg[1], Joel Abrahamson[2], Michael Strano[2], and Stephanie Reich[1] — [1]Department of Physics, Free University of Berlin, Berlin, Germany — [2]Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, USA

This contribution has been withdrawn.

MM 55: Topical Session Growth Kinetics V

Time: Thursday 14:00–15:15 Location: H4

MM 55.1 Thu 14:00 H4

Atomic scale simulations of silicon growth from the melt: Formation of twins and stacking faults studied by molecular dynamics and Monte Carlo methods — •Johan Pohl and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 32, D-64287 Darmstadt

Formation of twin boundaries and stacking faults at the silicon growth front is studied by lattice Monte Carlo and molecular dynamics (MD) simulations. First, we show how to construct a computationally efficient lattice-based Monte Carlo model that includes stacking faults and twin boundaries and allows to simulate crystal growth of large systems. Data on the importance of stacking faults for the roughening transition of the (111) interface and parallel twin growth velocities are extracted from the model.

In a further step, MD simulations reveal that twins do not nucleate on (111) microfacets in the perfect crystal, but exclusively occur in the vicinity of grain boundaries [1]. Only at an undercooling of 150 K we observe the formation of metastable twin bounded loops with incoherent interfaces to the matrix consisting of coherency and anticoherency dislocations. We conclude that the nucleation of stable twins in silicon growth requires the presence of a grain boundary or more general of a three-phase boundary, but is unlikely to occur on ideal (111) facets because of the excess energy of the interfacial area between matrix and twinned crystal.

MM 55.2 Thu 14:15 H4

Nutzung der Wachstumskinetik in Wandermagnetfeldern für die Czochralski-Züchtung von PV-Silizium mit quadratischem Querschnitt — •P. Rudolph[1], M. Czupalla[1], B. Lux[1] und F. Kirscht[2] — [1]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin — [2]CaliSolar GmbH, Berlin

Bei der Herstellung von Si-Solarzellen mit Standardkantenlängen von 125 bzw. 150 mm aus den zylindrischen Czochralski-Kristallen entstehen Präparationsverluste von 25-28%. Von Vorteil wäre das Ziehen von CZ-Kristallen mit quadratischem Querschnitt. Um die Verwendung kontaminierender Formgeber zu umgehen, kann man sich die kinetisch determinierte Ausbildung von seitenbegrenzenden Wachstumsfacetten zunutze machen. Wenn es gelingt sehr geringe radiale und zudem stabile Temperaturgradienten über den Tiegelradius einzustellen, wird der in [001]-Richtung gezogene Si-Kristall von vier {110}-Seitenflächen begrenzt. Nach Brice ist in einem konzentrischen Isothermenfeld die Facettenbreite $d = (2\Delta TR/G_T)^{1/2}$ mit R - Radius der Schmelzpunktisotherme, G_T - senkrecht dazu verlaufendem radialen Temperaturgradienten und ΔT - die für eine 2D-Keimbildung im Facettenzentrum erforderliche Unterkühlung. Mit einer spezifischen Heizer-Magnet-Konfiguration wird ein magnetisches Wanderfeld erzeugt, welches eine sehr stabile toroidale Strömung in der Schmelze mit extrem geringem G_T generiert. Bisher konnten reproduzierbar Si-Einkristalle solcher Querschnitte mit Kantenbreiten $d = 50 - 90$ mm gezogen werden. Strukturelle Perfektion, Sauerstoffgehalt und mikroskopische Morphologie der {110}-Facetten werden analysiert.

MM 55.3 Thu 14:30 H4

Minimum Energy Path for Nucleation with Phase Field Crystal — •Axel Voigt and Rainer Backofen — TU Dresden

Phase Field Crystal (PFC) is a well established model to study solidification in metals and colloids on an atomistic scale [1,2]. It can be connected to time dependent classical density functional theory. The time evolution of the density of particles is governed by a (at least) 6-th order partial differential equation. Thus, it is straight forward to calculate the time evolution of states, which is a minimization of total energy in the system. But, in order to study nucleation, the transition path between two (meta) stable states has to be explored. The nucleation barrier is then defined by the most probable transition path. This is equivalent to the minimum energy path (MEP). The MEP is the path in configuration space, where the driving force or dynamics of the system is parallel to the transition path [3]. Thus, the MEP allows us to identify saddle points which has to be overcome by nucleation as well as nucleation barriers. Recently a simplified string method was proposed in order to calculate MEP in high dimensional configuration spaces [3]. We will show the application of the simplified string method to nucleation in phase field crystal. Nucleation barriers as well as morphology of minimal stable nuclei will be discussed. Furthermore the influence of walls to nucleation will be shown.

[1] S. van Teeffelen, R. Backofen, A. Voigt and H. Loewen, Phys. Rev. E 79 051404 (2009) [2] R. Backofen, A. Raetz and A. Voigt, Phil. Mag. Let. 87 (11),(2007) [3] W. E, W. Ren and E. Vanden-Eijnden, J Chem. Phys. 126, 164103 (2007)

MM 55.4 Thu 14:45 H4

Role of Nucleation in Multi-Scale Phenomena of Solidification — •Abhik Choudhury and Britta Nestler — Institute of Materials and Processes, Moltkestrasse 30, Karlsruhe 76131

Solidification has been an interesting topic of study considering the vast scale of structures possible during the evolution of solids from an undercooled liquid. Considering their significance, it is worthwhile to get a basic understanding of the principles underlying the pattern formations, such that control mechanisms are possible to design their production. Epicentric are structures such as interdendritic lamellar eutectics and island banded and coupled growth morphologies in peritectic systems, which are principally formed as a result of interplaying multi-scale phenomena. Nucleation is understood to be an important phenomenon in maintaining scale of the eutectic lamellae in the case of interdendritic structures and the switching from island banded structures to coupled growth in some peritectic systems.

In the present study, we investigate the process of nucleation using the phase-field method. The presentation involves the calculation of the barrier to nucleation in eutectic and peritectic systems through the solution of the Euler-Lagrange(EL) equations which are formulated in the framework of the phase-field method. Special emphasis is placed on the description of a novel technique to solve the EL equations, based on an extension of the volume preservation method. The generality of the method allows for applications to a range of possible EL equations in material systems. The calculations are compared with phase-field simulations of nucleation with random noise.

MM 55.5 Thu 15:00 H4

Trapping effects on the critical nucleus size in nucleation a growth processes, kinetic Monte Carlo simulations — •Zoltan Balogh[1,2], Zoltan Erdelyi[2], and Dezso L Beke[2] — [1]Westfälische Wilhelms Universität-Münster, Institut für Materialphysik, Münster, Germany — [2]University of Debrecen, Department of Solid State Physics, Debrecen, Hungary

The critical nucleus size - above which a nucleus will grow and below dissolve - is calculated in a binary alloy during diffusion controlled phase separation using kinetic Monte Carlo simulations. In the calculations the differences in atomic mobilities are often neglected, however the difference of diffusion coefficients in a binary alloys can be as high as 4-8 orders of magnitude in technically important materials (like Si-Ge, Fe-Cr or Ni-Cu).

If the atomic jumps are slower in the A-rich nucleus than in the embedding B-rich matrix, the nucleus will trap the approaching A atoms to its surface. It has not enough time to reject them - despite this process would be favored thermodynamically - before new A atoms arrive. Thus the kinetic and thermodynamical critical size would be different for the nucleus. With reasonable trapping effect the former can be even an order of magnitude smaller than the latter.

MM 56: Topical Session Growth Kinetics VI

Time: Thursday 15:30–17:00 Location: H4

MM 56.1 Thu 15:30 H4

Computational analysis of interfacial attachment kinetics and transport phenomena during liquid phase epitaxy of mercury cadmium telluride

— Igal Rasin[1], Anne Ben Dov[2], Ilana Grimberg[2], Olga Klin[2], Eliezer Weiss[2], and •Simon Brandon[1] — [1]Dept. of Chemical Engineering, Technion, Haifa 32000, Israel — [2]SCD-Semi-Conductor Devices, P.O. Box 2250/99, Haifa 31021, Israel

Deposition of mercury cadmium telluride (MCT) thin films, on lattice matched cadmium zinc telluride substrates, is often achieved via Liquid Phase Epitaxy (LPE). The yield and quality of these films, required for the production of infrared detector devices, is to a large extent limited by lack of knowledge regarding details of physical phenomena underlying the deposition process. Improving the understanding of these phenomena and their impact on the quality of the resultant films is therefore an important goal which can be achieved through relevant computational and/or experimental studies.

We present a combined computational and experimental effort aimed at elucidating physical phenomena underlying the LPE of MCT via a slider growth process. The focus of the presentation will be results generated by a time-dependent three-dimensional model of mass transport, fluid flow, and interfacial attachment kinetics, which we have developed and applied in the analysis of this LPE process. These results, combined with experimental analyses, lead to an improved understanding of the role of different transport and kinetic phenomena underlying this growth process.

MM 56.2 Thu 15:45 H4

Zeolite thin film growth studied with a phase-field model

— •Frank Wendler, Christian Mennerich, and Britta Nestler — Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestr 30, 76133 Karlsruhe, Germany

Hydrothermally grown zeolite films are exeptionally interesting as molecular sieves, where the transport through the nanosized pores is strongly modulated by the grain orientation and boundary morphology. The objective of the simulation study is an understanding of the competitive growth behaviour and the formation of undesired mesoscale porosity during polycystalline growth to optimize process conditions. We adopt a multi-phase field model of Allen-Cahn type to describe the process, where each solid grain and the aquaeous solution are represented by individual order parameters. First, single coffin- or leaflet-shaped MFI zeolite crystals are modeled choosing appropriate anisotropies of surface tension and kinetic coefficient. Different aspect ratios and a transition between both crystal growth shapes emerge. Then, the selection dynamics is studied in simulations with several hundreds of grains in 2D and 3D, showing a gradual extinction according to misorientation and the influence of non-isotropic orientation distributions (seeded growth). The occurence and influence of growth twinning on the morphological evolution is discussed, which - similar to nucleation - produces new growth orientations during the process. Parts of the complex silicate chemistry are represented by taking into account the initially present gel phase (solution + amorphous solid), acting as a buffer layer in the transport of the silicate building blocks.

MM 56.3 Thu 16:00 H4

Combined phase-field and MD simulations of diffusion drop and ordering at $[\mathrm{Ni}_x\mathrm{Zr}_{1-x}]_{liquid}$-$\mathrm{Zr}_{crystal}$ interfaces

— •M. Guerdane, F. Wendler, and B. Nestler — Institute of Materials and Processes, Karlsruhe University of applied Sciences, Germany

We combine phase-field (PF) modeling and molecular dynamics (MD) simulations to show that the velocity of the solidification front in a two-phase $[\mathrm{Ni}_x\mathrm{Zr}_{1-x}]_{liquid}$-$\mathrm{Zr}_{crystal}$ structure is strongly affected by the drop of the liquid diffusion when approaching the solid-liquid interface. The latter is defined through a suitable order parameter that distinguishes between crystalline and liquid atomic environment. The diffusion drop near the interface is attributed to the pronounced short range order inherent to the $\mathrm{Ni}_x\mathrm{Zr}_{1-x}$ melt. The system transforms into a massive lateral ordering in the vicinity of the Zr crystalline wall. Our combined PF-MD analysis points out the shortcoming of the standard interpolation procedure, usually applied in constructing the phase dependent diffusivity, to describe the confinement effect caused by the crystalline wall at low temperatures.

MM 56.4 Thu 16:15 H4

The Interface of a Growing Zr-Ni Crystal

— •Philipp Kuhn and Jürgen Horbach — Deutsches Zentrum für Luft- und Raumfahrt, Institut für Materialphysik im Weltraum, Köln

Crystal growth of intermetallic phases in binary metallic alloys proceeds at a considerably slower pace than that of pure metals. As an example the growth in Zr-Ni is two orders of magnitude slower than that for pure Ni [1]. We perform molecular dynamics simulations of pure Ni and Zr-Ni systems to elucidate the mechanism behind this phenomenon. As an interaction model an embedded atom potential is used [2]. We utilize local order parameters to distinguish between solid and liquid particles and combine them in the form of two-dimensional maps [3] as a tool to analyze the structure of the layers in the interface region. This analysis serves as a prerequisite to determine the kinetics of mass transport in the interface region.

[1] H. Yasuda et al., J. Phys. **144**, 012056 (2009)

[2] T. Kumagai et al., Mat. Transact. **48** Nr. 6, pp. 1313–1321 (2007)

[3] W. Lechner and C. Dellago, J. Chem. Phys. **129**, 114707 (2008)

MM 56.5 Thu 16:30 H4

Conditions for the occurrence of Abnormal Grain Growth studied by a 3D Vertex Dynamics Model

— •Melanie Syha and Daniel Weygand — KIT, Institut für Zuverlässigkeit von Bauteilen und Systemen, Kaiserstr. 12, 76128 Karlsruhe

The three dimensional (3D) vertex dynamics model presented in [1,2] has proven to be suited to model the coarsening of systems of up to several thousand grains with an excellent agreement to the MacPherson/Srolovitz relation for the volume change rate. Now this model is applied to investigate the phenomenon of Abnormal Grain Growth (AGG) in SrTiO3.Although the effect of AGG in perovskite materials in absence of pinning is covered by several investigations [3,4] the underlying mechanisms are still not well understood.In contrast to classical mean field approaches which often assume special but uniform GB properties for the abnormally growing grain of size r, the present study focusses on the role of GB mobility and energy variation, such as inclination dependencies, on the onset of AGG. [1] M. Syha, D. Weygand, A generalized vertex dynamics model for grain growth in three dimensions, accepted for publication, Modeling Simul. Mater. Sci. Eng. [2] D. Weygand, Y. Bréchet, J. Lépinoux, W. Gust, Three dimensional grain growth: A vertex dynamics simulation,Phil. Mag. B 79 (1999) 703-16 [3] T. Sano, G. Rohrer, Experimental evidence for the Development of Bimodal Grain Size Distributions by the Nucleation-Limited Coarsening Mechanism, J. Am. Ceram. Soc. 90 (2007) 199-204 [4] C. Bae, J. Park, Y. Kim, H. Jeon, Abnormal Grain Growth of Niobium-Doped Strontium Titanate, J. Am. Ceram. Soc. 81 (1998) 3005-09

MM 56.6 Thu 16:45 H4

Twist grain boundary migration by molecular dynamics simulation

— •Volker Mohles, Jian Zhou, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany

Molecular dynamics (MD) simulations with EAM potentials were used to study grain boundary migration of [001], [110] and [111] twist grain boundaries (GBs) in aluminum. The motion of GBs was driven by a crystal orientation dependent driving force. During GB migration, all GBs were found to be flat and to retain their structures at a given temperature. The GB structure was found to vary depending on temperature and the misorientation angle, and to be crucial for GB mobility. For some high-angle high-energy GBs, a transition from a solid-like structure to a liquid-like one was observed at elevated temperatures. This transition affects GB migration significantly. Our simulations yield twist GB mobility data in conspicuous agreement with those derived from real experiments.

MM 57: Topical Session Battery Materials III

Time: Thursday 14:00–15:30 Location: H6

Topical Talk MM 57.1 Thu 14:00 H6

Physical properties and synthesis of thin film materials for batteries — •Nancy Dudney — Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Thin film batteries prepared by vapor deposition processes are being manufactured for a variety of devices. These small power sources offer extended cycle life and stability under extremes in temperature and charging conditions. With a planar structure and chemistry free of side reactions and sei formation, the thin film batteries can also be used as a model test cell for exploring the transport and physical properties of battery materials and interfaces. Examples will be described as well as recent efforts focused on developing processing for 3D architectures.

Acknowledgement: This research was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy.

MM 57.2 Thu 14:30 H6

Li ion transport in sputter deposited $LiCoO_2$ thin films and glassy borate membranes — •Tobias Stockhoff, Tobias Gallasch, and Guido Schmitz — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Münster (Westf.), Germany

$LiCoO_2$ membranes are key components of current battery technology. We investigate sputter-deposited thin films of these materials aiming at the application in all-solid-state thin film batteries. For this, $LiCoO_2$ films (10 - 200 nm) were deposited onto ITO-coated glass substrates by ion beam sputtering. In addition, a part of these films are coated by an ion-conductive membrane of Li_2O-B_2O_3 glasses in the thickness range of 50 to 300 nm. Structural, chemical and electrical properties of the layers are studied by means of TEM (EELS) and various electrical methods (cyclic voltammetry, chrono-amperometry / -potentiometry).

Since the color of the $LiCoO_2$ films changes from red-brown to grey during de-intercalation of Li and the substrate as well as the glassy membrane deposited on top are optical transparent, reversible Li de- and intercalation can be directly demonstrated and quantified by a measurement of light transmission through the layered system. Samples coated with an ion-conductive membrane reveal a characteristic delay in switching optical transparency which is due to the slower transport across the membrane. Varying the thickness of the glassy membrane, the d.c. ion-conductivity and permeation through the membrane is determined quantitatively. Using thin membranes in the range of a few tens of nanometers the critical current densities are way sufficient for battery applications.

MM 57.3 Thu 14:45 H6

Electron energy loss spectroscopy of thin film electrodes and membranes in all-solid-state batteries — •Tobias Gallasch, Dietmar Baither, and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Electron energy loss spectroscopy (EELS) is based on inelastic scattering of electrons in the TEM. The technique allows evaluating the chemical composition, the oxidation states and therefore, also the bonding characteristics of layered samples with a spatial resolution in the nanometer range.

For the experiments, model batteries comprising of layers of $LiCoO_2$, Li-Borate glasses and V_2O_5 are deposited onto ITO-coated glass substrates. Single layer thickness ranges from 50 to 400 nm. Electron transparent cross section samples are prepared by conventional ion milling and FIB technique. Measuring the observed chemical shift in the absorption edges of the energy loss spectra and comparing these to appropriate reference materials, different charge states of the electrodes can be distinguished and the amount of Li intercalated in the structure is quantified. The talk demonstrates how these data are used to optimize the conditions of sputter deposition and to achieve suitable functional properties of the thin films.

Reversible Li-intercalation in the model thin film battery with active layers of 200 nm thickness and 50 nm thick membranes is demonstrated by cyclic voltametry.

MM 57.4 Thu 15:00 H6

Grenzflächen-Untersuchungen an Festkörper-Batterien — •Susanne Jacke, Jie Song, Gennady Cherkashinin, René Hausbrand und Wolfram Jagermann — TU Darmstadt, Fachbereich Materialwissenschaft, Petersenstrasse 32, 64287 Darmstadt

Dünnschicht-Festkörperbatterien sind in letzter Zeit in den Fokus verschiedener Forschungsaktivitäten für Anwendungen in mobilen elektronischen Geräten sowie Mikroelektronik oder Solarzellen gerückt. Ein wichtiger Aspekt bei der Verbesserung der Eigenschaften dieser Batterien ist das Verständnis der Ermüdungserscheinungen. Bei dem Zyklieren der Batterien spielen die Grenzflächen zwischen Elektrolyt und Elektroden eine wichtige Rolle. In der vorliegenden Studie wurde die Entstehung von Festkörper-Festkörper Grenzflächen schon während des Aufwachsprozesses der Batterie in der Herstellung untersucht. So wurde die Entstehung der Grenzschicht zwischen Kathode und Elektrolyt sowie die zwischen Anode und Elektrolyt untersucht, indem ihre Zusammensetzung nach kurzen Depositionsschritten mit Photoelektronenspektroskopie analysiert wurde. Die Kathode, bestehend aus LiCoO2, wurde mit Hilfe von Sputter-Deposition aufgebracht, ebenso wie der LiPON- Elektrolyt und die Lithium-Aluminium-Anode. Eine auf diese Weise hergestellte Batterie zeigte das charakteristische Zyklierungsverhalten einer Batterie. Einige interessante Abweichungen von der Festkörperstruktur wurden an der Grenzfläche gefunden: so entsteht z.B. an der Grenzfläche Elektrolyt-Kathode eine Zwischenschicht, die Nitrit- (NO2)-, und Nitrat (NO3)- Produkte enthält.

MM 57.5 Thu 15:15 H6

Valence states and surface/interface reactions in Li-ion battery cathodes — •Gennady Cherkashinin[1], David Ensling[1], Stefan Schmid[1], Jie Song[1], Susanne Jacke[1], Renè Hausbrand[1], Kristian Nikolowski[2], Helmut Ehrenberg[2], and Wolfram Jaegermann[1] — [1]Department of Materials Science, Surface Science Institute, Darmstadt University of Technology, Darmstadt 64283, Germany — [2]IFW Dresden, Institute for Complex Materials, Germany

Surface electronic properties of promising Li-Ion cathode materials such as LiMO2 (Ni, Co, Mn) as well as evolution of electrolyte-cathode interfaces formed after contact to the electrolyte, due to electrochemical charging and after cycling were systematically studied using XPS, UPS and synchrotron photoelectron spectroscopy (SXPS, XAS). To study fundamental surface properties of the oxides we investigated both thin film cathodes in-situ, whose surfaces are not contaminated by impurities, and synthesized powder cathodes used in industry. For LiMO2 (Ni, Co, Mn) cathodes, we have found that contact of the cathodes to the electrolyte results in the loss of lattice lithium and in the formation of a solid electrolyte interface (SEI) layer consisting of Li2CO3, LixOy, LiF (if LiPF6-electrolyte is used) and other species. For oxides containing Ni3+, we observe a Ni3+ to Ni2+ reduction. Charging of Lix(M)O2 (M=Co,Ni) does not only lead to Co3+ to Co4+ oxidation but also to oxygen deficiency. We detect no oxygen site participation in the charge compensation at the initial stage of the Li-de-intercalation.

MM 58: Topical Session Battery Materials IV

Time: Thursday 15:45–17:30 Location: H6

Topical Talk MM 58.1 Thu 15:45 H6

Investigation of Microscopic Mechanisms and Mechanical Effects in Electrode Materials for Lithium-Ion Batteries — •Reiner Mönig — Karlsruhe Institute of Technology, Institute for Materials Research II, Postfach 3640, 76021 Karlsruhe, Germany

Lithium ion batteries are promising candidates for future electrical energy storage. Important components of batteries are the electrodes which critically determine energy and power density as well as reliability. In the electrodes, sufficiently high ionic and electronic conductivities often can only be achieved by using small particles. The small particles, which are often in the 100nm range, make detailed investigates complicated. For example, typical electrochemical characterization methods can only yield volume averaged data of a whole electrode. In this talk a technique for in situ scanning electron microscopy will be introduced. Observations recorded during Lithium insertion and extraction into individual Si nanowires and SnO_2 particles will be presented. The experiments give insight into the fundamental processes that control battery operation and reveal degradation mechanisms. Large volume expansions and the growth of cracks were frequently observed. In order to assess mechanical stresses arising from Li insertion/extraction, dedicated in situ substrate curvature experiments were performed. Mechanical stress seems to be an important factor controlling battery operation and degradation. In contrast to many chemical degradation mechanisms that can be suppressed by chemical means, mechanical stresses are inevitable and their consequences may be limiting factors for the applicability of novel battery materials.

MM 58.2 Thu 16:15 H6

Microscaopic investigation of Li-Ion Batteries and Quantitative Characterization of the Microstructure — •Carmen Hafner, Timo Bernthaler, Alwin Nagel, and Gerhard Schneider — Aalen University, Department Materials Science and Surface Engineering, Aalen, Germany

Lithium ion batteries are the most attractive candidates for mobile applications. The function of Li ion batteries is based on the change of active materials due to diffusion processes. Electrochemical and physical characterization techniques are well advanced and published. Unlike these techniques the microscopic visualization and quantification of the microstructure of the electrode materials are not state of the art. Cell performance and aging mechanisms depend strongly on the appearance and changes in the microstructure. Hence, the investigation and quantification of microstructures is of increasing importance for the understanding of battery materials. We present the potential of the combined microscopic techniques nano 3D-computed tomography, optical microscopy, scanning electron microscopy and image analysis to characterize cell designs and the microstructure of active materials. The process how to prepare and investigate Li ion batteries by these techniques will be described. For the measurement of specific microstructural features of the active materials methods of the quantitative microstructure analysis will be explained. Parameters like volume fraction of phases, homogeneity, pores, cracks, grain size and shape distribution and specific surfaces and interfaces will be discussed.

Topical Talk MM 58.3 Thu 16:30 H6

New materials for energy storage systems — •Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Baden-Württemberg, Ulm

Electrochemical energy storage systems are the key components for mobile applications both in communication systems and in new car concepts as hybrid or full electric vehicles. The rechargeable lithium-ion battery system has become the dominant technology in the global battery market during the last decade. These batteries offer the highest energy density available to date. While commercially used lithium-ion batteries power mostly small devices as cellular phones, portable computers and other mobile electronic equipment, extensive world wide efforts are underway to develop this technology for much more demanding applications such as large batteries for electric vehicles.

The present status of rechargeable lithium-ion batteries, the requirements for various applications and the need for further development will be discussed. The focus of the presentation deals with the materials selection and the materials science principles that underlie the behaviour of advanced electrochemical storage systems. An overview of current electrode materials (anode and cathode) and electrolytes will be given and future research and development needs for new components will be discussed.

MM 58.4 Thu 17:00 H6

Metallocene-based nanocomposites as cathode materials in lithium batteries — •Raju Prakash, Clemens Wall, and Maximilian Fichtner — Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Lithium-ion batteries have been the most utilized batteries in the portable electronic market since many years. But their performance still lies behind the demands of the consumer. New electrode materials with high specific capacities are necessary to meet these demands. Metal fluorides have high theoretical specific capacity based on a novel conversion mechanism, making them promising cathode materials for high performance lithium-ion batteries. However, the metal fluoride cathodes are still hampered by loss of capacity and cyclic instability. Hence, a new approach such as encapsulation of active materials in nanotubes or carbon-coating, etc. is needed in order to improve their performance.

Herein, we present a simple method based on the thermal decomposition of a metallocene/LiF mixture to produce inexpensive cathode materials which exhibit a good cyclic stability and reversibility. The detailed structural investigations of the nanocomposites as well as their electrochemical performances will be presented.

MM 58.5 Thu 17:15 H6

The *ortho*–phosphate arrojadite as new material for cathodes in Lithium–ion batteries. — •Christoph Kallfass[1], Constantin Hoch[1], Hermann Schier[1], and Helmut Schubert[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisernbergstr. 1, D-70569 Stuttgart, — [2]Technische Universität Berlin, Institut für Werkstoffwissenschaften, Englische Str. 20, D-10587 Berlin

The investigation of the crystal structure of the iron- and manganese containing *ortho*–phosphate mineral arrojadite was extending over several years [1-3]. Single crystal diffraction using X–ray and neutron radiation combined with complete determination of all chemical constituents of the component result in a new structural model. The new model describes two different types of channels running along [010] and elucidates the occupancy of the atomic positions inside these channels. A novel chemical process offers the opportunity to modify the the elementar arrangement of the atomic positions inside the channels using methods of so–called “green chemistry”. When using Li^+ cations in this process a new material for cathodes can be made out of the mineral arrojadite. A lithium–ion battery made of an arrojadite cathode worked for more than 15.000 cycles ($2.0 \leq V \leq 4.5$) with minor loss in capacity. The novel chemical process and particularly the enrichement of Li^+ cations was verified by single crystal diffraction using neutron radiation and ^{6}Li–MAS–NMR–spectroscopy.

[1] Krutik, V. M. *et al. Sov. Phys. Crystallogr.*, **24**, 425–429, 1979.
[2] Moore, P. B. *et al. Am. Mineral.*, **66**, 1034–1049, 1981.
[3] Cámara, F. *et al. Am. Mineral.*, **91**, 1249–1259, 2006.

MM 59: Phase Transitions I

Time: Thursday 14:00–15:15 Location: H5

MM 59.1 Thu 14:00 H5

The Phase Diagram of Iron Clusters: A molecular Dynamics Study — •Denis Comtesse[1], Ralf Meyer[2], and Peter Entel[1] — [1]Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Laurentian University, Sudbury, Ontario, P3E 2C6 Canada

The stability of phases at finite temperatures is given by the free energy. But the fact that it is not expressible in terms of ensemble averages over functions of position and velocity coordinates, complicates its determination in atomistic simulations. In order to overcome this problem, thermodynamic integration methods are used. This method is not limited to thermodynamic paths which can be followed in experiments. Often artificial paths along which the inter-particle interaction is switched off, lead to much better results.

Here we calculate the free energy of iron nano clusters along a thermodynamic path starting from the embedded atom model and ending up in a set of three dimensional harmonic oscillators. The results allow to arrange the various morphologies in a phase diagram of temperature and number of atoms. The phase boundaries, which are normally hidden in between hysteresis loops, can be determined very accurately from the intersection of the free energies of the competing morphologies. As examples, we analyse three common morphologies, namely the icosahedron, the cuboctahedron with fcc structure and its Bain transformation to the bcc structure. Additionally the new shellwise

Mackay transformed morphology reported in Phys. Rev. Lett. **99** 083402 is taken into account.

MM 59.2 Thu 14:15 H5

Bulk and near-surface microstructure of Ni-23 at.% Pt — •Markus Engelke[1], Bernd Schönfeld[1], and Andrei Ruban[2] — [1]LMPT, Department of Materials, ETH Zurich — [2]KTH Stockholm, Sweden

Diffuse x-ray scattering was taken from bulk single-crystalline Ni-23.2 at.% Pt. The sample was aged at 923 K to set up a state of thermal equilibrium. Using separation techniques, short-range order and static atomic displacements were determined. In comparison with a previously performed study from the same sample to characterize the near-surface microstructure by grazing incidence diffraction, differences are noted: they mainly refer to the static atomic displacements, being smaller in magnitude in the bulk than in the near-surface region. Effective pair interaction parameters show a dominant nearest-neighbor parameter, larger than that on the Pt-rich side. This is reflected in different order-disorder transition temperatures for Ni with 25 and 75 at.% Pt ($L1_2$ structure). First-principles electronic structure calculations support these findings.

MM 59.3 Thu 14:30 H5

Bonding in boron: building high-pressure phases from boron sheets — •Jens Kunstmann[1], Lilia Boeri[2], and Jens Kortus[3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Institute for Theoretical Physics, TU Bergakademie Freiberg, Germany

We present the results of a study of the high pressure phase diagram of elemental boron, using full-potential density functional calculations. We show that at high pressures ($P > 100$ GPa) boron crystallizes in quasi-layered bulk phases, characterized by in-plane multicenter bonds and out-of-plane unidimensional sigma bonds. These structures are all metallic, in contrast to the low-pressure icosahedral ones, which are semiconducting. We show that the structure and bonding of layered bulk phases can be easily described in terms of single puckered boron sheets [1]. Our results bridge the gap between boron nanostructures and bulk phases. [1] Kunstmann et al., Phys. Rev. B 74, 035413 (2006).

MM 59.4 Thu 14:45 H5

Memory Effects in Confined Fluids via Diffusion Measurement — •Sergej Naumov, Rustem Valiullin, and Jörg Kärger — Universität Leipzig, Fak. Phys, u. Geowiss., Linnestr. 5, 04105, Deutschland

The detailed knowledge about the molecular transport in nanoporous materials is of enormous importance for the industrial applications. The transport of molecules in the nanopores can be affected by gas-liquid phase transitions. The latter are often accompanied by adsorption hysteresis, i.e., the concentration of the molecules inside the pores depends not only on the external parameters like gas pressure or temperature, but also on the history how the external parameters have been varied. The evolution of the fluid state may be probed by means of Pulsed Field Gradient NMR which can trace the amount adsorbed simultaneously with the self-diffusion coefficients of the molecules [1]. The thus obtained self-diffusivities are found to depend not only on fluid concentration, but also on the history how a particular concentration has been attained [2].

[1] Naumov, S.; Valiullin, R.; Monson, P. A.; Kärger, J., Langmuir, 2008, 24, 6429-6432

[2] Valiullin, R.; Naumov, S.; Galvosas, P.; Kärger, J.; Woo, H.; Porcheron, F.; Monson, P. A. Nature, 2006, 443, 965-968

MM 59.5 Thu 15:00 H5

Microstructure simulations of porous media, of cell motion in flow fields and the interaction with structured surfaces — •Britta Nestler, Ali Aksi, Michael Selzer, Marcus Jainta, and Frank Wendler — Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

A Lattice-Boltzmann method for modelling fluid flow is coupled with the dynamic equations of a phase-field model for phase transformations and microstructure evolutions in multiple order parameter systems. The model contains a formulation for phases with preserved volume fractions and an extension for considering pressure differences in the various phase regions. The combined approach is applied to dry and wet foams and to computationally evaluate the permeability and microporosity in porous media. At the phase boundaries, we employ a smooth formulation of a bounce-back condition related to the diffuse interface profile. Simulations of fluid flow in static porous media with stationary non-moving interfaces and in microstructures performing a dynamic evolution of the boundaries are presented. We further study the motion of particles in a shear flow and measure the effective viscosity of the fluid for different particle distributions, channel geometries, volume fractions and properties of the fluid. The method is also capable to investigate the behaviour of liquid droplets on top of structured surfaces. The results are compared with experiments related to the Lotus effect for different surface energies and contact angles in the presence and absence of fluid flow.

MM 60: Phase Transitions II

Time: Thursday 15:30–17:00 Location: H5

MM 60.1 Thu 15:30 H5

Colloidal model systems for undercooled metallic melts — •Ina Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Thomas Palberg[2], 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, 55128 Mainz, Germany

Due to their mesoscopic length scales, colloidal suspensions are ideal model systems to address fundamental issues in condensed matter physics such as liquid ordering, nucleation and crystallization. Colloidal particles are several orders of magnitude larger than atoms in metals and their relaxation behavior is very sluggish compared to atomic systems. Due to the possibility of tunable interaction, systematic investigations of the short-range order in a charged colloidal silica system far from equilibrium state are presented. Therefore, time-dependent structure factors in the undercooled state were measured applying Ultra Small Angle X-ray Scattering. The results of these investigations are compared to measurements on metallic systems represented by an undercooled Ni melt applying neutron scattering. The measured structure factors of both physically different systems are analyzed using the same evaluation method which reveals icosahedral short-range order in the melt phase of both systems, colloids and pure metals as well. In addition, due to the variation of the interaction potential from soft repulsive to hard-sphere like bahavior, icosahedral short-range order is replaced by a fcc structure near the solid-fluid phase boundary.

MM 60.2 Thu 15:45 H5

Crystallization in a model system of charged colloidal particles: How do larger particles influence the crystallization process and therefore the resulting microstructure? — •Andreas Engelbrecht and Hans Joachim Schöpe — Johannes Gutenberg-University, 55099 Mainz, Germany

Characteristics of a material often depend on the microstructure of the material (i.e. the grain size in metals,) therefore the control of the crystallization process allows access to new materials of desired properties. Colloidal suspensions of spherical particles are widely used as model system for molecular and atomic systems - especially for metals. Progress understanding the solidification process has been made in recent years studying colloidal suspensions.

The formation of crystals from the melt can be controlled either by the required activation energy or by the rate of particles attaching to the crystal liquid interface. Adding just small amounts (less than 1%) of a larger and higher charged spherical particles to colloidal suspension of charged spheres we observe a drastic variation of the crystallization process and for this reason the resulting microstructure of the solidified material is changing its appearance. Expressed in terms of the classical nucleation theory the observed enormous effect on crystal nucleation is not exclusively induced by a significant change of the nucleation barrier height, but by a modification of the kinetic prefactor. A variation in the transport mechanism of particles form the melt towards the crystals modifies the kinetic prefactor of the classical nucleation theory as well as the crystal growth.

MM 60.3 Thu 16:00 H5

Competition between heterogeneous and homogeneous nucleation near a flat wall — Andreas Engelbrecht, Roushdey Salh, and •Hans Joachim Schöpe — Johannes Gutenberg-University, 55099 Mainz, Germany

The physical and chemical properties of solidified crystalline materials depend in a crucial way from the conditions of crystal nucleation. In order to improve the conditions of production processes and even to develop novel materials with extraordinary properties a detailed knowledge of the nucleation process is most desired.

We studied the competition between heterogeneous and homogeneous nucleation in colloidal model systems of charged spheres close to the container walls as function of metastability.

Our results show some unexpected behaviour: Although the appearing polycrystal displays a high amount of wall crystal we find that the heterogeneous nucleation at the container walls is delayed in comparison to the homogeneous bulk nucleation and its rate density appears surprisingly slightly smaller demonstrating the complexity of the observed crystallization process.

MM 60.4 Thu 16:15 H5

Bulk liquid undercooling and nucleation in Nickel — •Joachim Bokeloh, Anna Moros, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

While classical nucleation theory is widely accepted textbook knowledge, it is somewhat lacking with regard to the atomistic details of the nucleation and growth mechanisms. Right now, there are many efforts in exploring these details with computational methods. However, only few experimental methods that can corroborate these results are available. The best known of these experimental methods are containerless processing in levitation melting and the investigation of fine droplet dispersions.

We present here data on the liquid undercooling behaviour of Ni obtained by repeated melting and crystallization in a DTA. This method allows to acquire a statistically meaningful data set under clean and reproducible conditions, while still allowing reasonable sample sizes, thus combining several advantages of the two methods mentioned above. Ni was chosen as a model system because it shows good levels of undercooling and because it is well suited for computer simulations due to its relatively low number of electrons.

MM 60.5 Thu 16:30 H5

Investigation of nucleation in undercooled metal melts — •Stefan Klein[1,2] and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 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 7 mm are processed within high purity inert gas atmosphere while in case of electrostatic levitation samples in a diameter of 2 mm 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 60.6 Thu 16:45 H5

Neural Network Potential-Energy Surfaces for Materials Simulations — Nongnuch Artrith, Tobias Morawietz, and •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Artificial neural networks represent a very flexible class of mathematical functions, which is well suited for the construction of potential-energy surfaces by interpolating a set of reference energies obtained from accurate electronic structure calculations. Recently, the applicability of neural network potentials has been extended to high-dimensional energy surfaces of condensed systems. By incorporating long-range electrostatic interactions also multicomponent systems can be addressed. Using semiconductors, oxides and metals as benchmark systems we show that neural networks provide reliable potentials for a wide range of materials. Since analytic gradients are readily available to calculate the forces, neural network potentials can be used to carry out efficient molecular dynamics simulations.