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Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks and Sessions

(Lecture Rooms H4, H24, H25 and H26; Poster E)

Invited Talks

MM 1.1	Mon	9:30–10:00	H24	**New opportunities and challenges in chromatic aberration corrected and in situ transmission electron microscopy** — •Rafal E. Dunin-Borkowski, Lothar Houben, Juri Barthel, Andreas Thust, Chris Boothroyd, Martina Luysberg, Andras Kovacs, Martial Duchamp, Joachim Mayer
MM 6.1	Mon	11:45–12:15	H4	**Prospects for mapping spins with atomic resolution in TEM** — •Johan Verbeeck
MM 6.2	Mon	12:15–12:45	H4	**Structural Characterization of nc-Si / SiO_x based quantum superstructures for the solar cell application by aberration-corrected high resolution electron microscopy** — •Maryam Beig Mohamadi, Birger Berghoff, Joachim Mayer
MM 10.1	Mon	15:00–15:30	H24	**Materials Science and Development of Complex Materials** — •Jan Schroers
MM 16.1	Tue	9:30–10:00	H24	**Combinatorial approach to multifunctional materials** — •Ichiro Takeuchi
MM 29.1	Wed	9:30–10:00	H24	**Modelling and understanding the strength of grain boundaries based on ab-initio results** — •Rebecca Janisch
MM 46.1	Wed	18:00–18:30	H24	**Brittle-ductile transitions - cracks and dislocations** — •Steve Roberts
MM 47.1	Wed	18:30–19:00	H24	**Microscopic friction mechanisms on metal surfaces** — •Roland Bennewitz
MM 48.1	Thu	9:30–10:00	H24	**Hydrogen embrittlement revisited by novel nano-mechanical approach** — •Afrooz Barnoush, Mohammad Zamanzade, Masoud Asgari, Roy Johnsen, Horst Vehoff
MM 57.1	Thu	15:00–15:30	H24	**Micro- and macroplastic behavior of nanocrystalline Pd-Ag alloy in temperature range between 4 and 300K** — •Yulia Ivanisenko

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H24	**Invited Talk (Hauptvortrag): Dunin-Borkowski**
MM 2.1–2.3	Mon	10:15–11:30	H4	**Topical Session: TEM-Symposium - Joint Session with MI I**
MM 3.1–3.5	Mon	10:15–11:30	H24	**Computational Materials Modelling - Fundamentals**
MM 4.1–4.3	Mon	10:15–11:30	H25	**Topical Session: Quasicrystals & Complex Metallic Alloys I**
MM 5.1–5.5	Mon	10:15–11:30	H26	**Functional Materials - Battery Materials I**
MM 6.1–6.4	Mon	11:45–13:15	H4	**Topical Session: TEM-Symposium - Joint Session with MI II**
MM 7.1–7.5	Mon	11:45–13:00	H24	**Computational Materials Modelling - Methods**
MM 8.1–8.4	Mon	11:45–13:00	H25	**Topical Session: Quasicrystals & Complex Metallic Alloys II**
MM 9.1–9.5	Mon	11:45–13:00	H26	**Functional Materials - Battery Materials II**
MM 10.1–10.1	Mon	15:00–15:30	H24	**Invited Talk (Hauptvortrag): Schroers**
MM 11.1–11.9	Mon	15:45–18:15	H4	**Topical Session: TEM-Symposium - STEM**

MM 12.1–12.10	Mon	15:45–18:15	H24	**Computational Materials Modelling - Mechanical Properties**
MM 13.1–13.9	Mon	15:45–18:00	H25	**Topical Session: Quasicrystals & Complex Metallic Alloys III**
MM 14.1–14.10	Mon	15:45–18:15	H26	**Functional Materials - Hydrogen**
MM 15.1–15.86	Mon	18:00–20:00	Poster E	**Poster Session**
MM 16.1–16.1	Tue	9:30–10:00	H24	**Invited Talk (Hauptvortrag): Takeuchi**
MM 17.1–17.4	Tue	10:15–11:30	H4	**Topical Session: TEM-Symposium - HR Imaging & Analytic I**
MM 18.1–18.5	Tue	10:15–11:30	H24	**Computational Materials Modelling - Phase Stability I**
MM 19.1–19.3	Tue	10:15–11:30	H25	**Topical Session: Combinatorial Materials Science I**
MM 20.1–20.5	Tue	10:15–11:30	H26	**Transport & Diffusion I**
MM 21.1–21.4	Tue	11:45–13:00	H4	**Topical Session: TEM-Symposium - HR Imaging & Analytic II**
MM 22.1–22.5	Tue	11:45–13:00	H24	**Computational Materials Modelling - Phase Stability II**
MM 23.1–23.4	Tue	11:45–13:00	H25	**Topical Session: Combinatorial Materials Science II**
MM 24.1–24.5	Tue	11:45–13:00	H26	**Transport & Diffusion II**
MM 25.1–25.3	Tue	15:00–16:00	H4	**Topical Session: TEM-Symposium - Structure-Property**
MM 26.1–26.4	Tue	15:00–16:00	H24	**Computational Materials Modelling - Diffusion & Kinetics I**
MM 27.1–27.2	Tue	15:00–16:00	H25	**Topical Session: Combinatorial Materials Science III**
MM 28.1–28.4	Tue	15:00–16:00	H26	**Transport & Diffusion III**
MM 29.1–29.1	Wed	9:30–10:00	H24	**Invited Talk (Hauptvortrag): Janisch**
MM 30.1–30.5	Wed	10:15–11:30	H4	**Topical Session: Fundamentals of Fracture - Modelling Intergranular Fracture**
MM 31.1–31.5	Wed	10:15–11:30	H24	**Computational Materials Modelling - Diffusion & Kinetics II**
MM 32.1–32.4	Wed	10:15–11:30	H25	**Topical Session: TEM-Symposium - Structure-Property / In-Situ I**
MM 33.1–33.5	Wed	10:15–11:30	H26	**Structural Materials**
MM 34.1–34.5	Wed	11:45–13:00	H4	**Topical Session: Fundamentals of Fracture - Fracture at the Atomistic Scale**
MM 35.1–35.5	Wed	11:45–13:00	H24	**Computational Materials Modelling - Phonons & Phase Stability**
MM 36.1–36.4	Wed	11:45–13:00	H25	**Topical Session: TEM-Symposium - Structure-Property / In-Situ II**
MM 37.1–37.5	Wed	11:45–13:00	H26	**Mechanical Properties I**
MM 38.1–38.4	Wed	15:00–16:15	H4	**Topical Session: Fundamentals of Fracture - Atomistic Modelling**
MM 39.1–39.5	Wed	15:00–16:15	H24	**Computational Materials Modelling - Transport, Excitations, Time Dependence I**
MM 40.1–40.4	Wed	15:00–16:15	H25	**Topical Session: TEM-Symposium - In-Situ I**
MM 41.1–41.5	Wed	15:00–16:15	H26	**Mechanical Properties II**
MM 42.1–42.4	Wed	16:30–17:45	H4	**Topical Session: Fundamentals of Fracture - Continuous Models**
MM 43.1–43.5	Wed	16:30–17:45	H24	**Computational Materials Modelling - Transport, Excitations, Time Dependence II**
MM 44.1–44.4	Wed	16:30–17:45	H25	**Topical Session: TEM-Symposium - In-Situ II**
MM 45.1–45.5	Wed	16:30–17:45	H26	**Nanomaterials - Nanospheres & Fibres**
MM 46.1–46.1	Wed	18:00–18:30	H24	**Invited Talk (Hauptvortrag): Roberts**
MM 47.1–47.1	Wed	18:30–19:00	H24	**Invited Talk (Hauptvortrag): Bennewitz**
MM 48.1–48.1	Thu	9:30–10:00	H24	**Invited Talk (Hauptvortrag): Barnoush**
MM 49.1–49.4	Thu	10:15–11:30	H4	**Topical Session: Fundamentals of Fracture - Novel Experimental Techniques I**
MM 50.1–50.5	Thu	10:15–11:30	H24	**Computational Materials Modelling - Defects & Interfaces I**
MM 51.1–51.5	Thu	10:15–11:30	H25	**Nanomaterials - Nanocrystalline & Porous Materials I**
MM 52.1–52.5	Thu	10:15–11:30	H26	**Phase Transformations I**
MM 53.1–53.5	Thu	11:45–13:00	H4	**Topical Session: Fundamentals of Fracture - Novel Experimental Techniques II**
MM 54.1–54.5	Thu	11:45–13:00	H24	**Computational Materials Modelling - Defects & Interfaces II**
MM 55.1–55.5	Thu	11:45–13:00	H25	**Nanomaterials - Nanocrystalline & Porous Materials II**
MM 56.1–56.5	Thu	11:45–13:00	H26	**Phase Transformations II**
MM 57.1–57.1	Thu	15:00–15:30	H24	**Invited Talk (Hauptvortrag): Ivanisenko**
MM 58.1–58.4	Thu	15:45–17:00	H4	**Topical Session: Fundamentals of Fracture - Fatigue Fracture**
MM 59.1–59.5	Thu	15:45–17:00	H24	**Computational Materials Modelling - Phase Stability III**

MM 60.1–60.5	Thu	15:45–17:00	H25	**Nanomaterials - Nanoparticles**
MM 61.1–61.5	Thu	15:45–17:00	H26	**Liquid & Amorphous Metals I**
MM 62.1–62.5	Thu	17:15–18:45	H4	**Topical Session: Fundamentals of Fracture - Stochastic Aspects**
MM 63.1–63.7	Thu	17:15–19:00	H24	**Computational Materials Modelling - Phase Stability IV**
MM 64.1–64.6	Thu	17:15–18:45	H25	**Nanomaterials - Miscellaneous**
MM 65.1–65.7	Thu	17:15–19:00	H26	**Liquid & Amorphous Metals II**

Topical session "Fundamentals of Fracture"

Organizers: Prof. Dr. Erik Bitzek (Universität Erlangen-Nürnberg), Prof. Dr. Sandra Korte (Universität Erlangen-Nürnberg), Prof. Dr. Peter Gumbsch (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg)

This symposium is intended as an international forum for the presentation and discussion of the latest scientific developments related to fundamental mechanisms and physics of fracture. The general theme of the Fundamentals of Fracture Symposium is to cover all aspects of fracture at a fundamental level, rather than specific engineering approaches. We aim at bringing together specialists from the fields of solid state physics, materials science, continuum mechanics, statistical physics and mathematics.
The symposium will cover theory, multi-scale modelling and recent experimental advances related to interaction of cracks with the microstructure, interplay of fracture and plasticity, initiation of fracture, fracture of nanostructures and -materials, influence of constraints on fracture, fracture of disordered materials, Statistical aspects of fracture, dynamic fracture, environmental effects on fracture.

Topical session "TEM-Symposium: Using Transmission Electron Microscopy to Unravel the Mysteries of Materials"

Organizers: Prof. Cynthia A. Volkert (Universität Göttingen), Prof. Dr. Joachim Mayer (RWTH Aachen)

Recent advances in transmission electron microscopy have led to significant improvements in spatial and energy resolution, and have also prompted the development of new tools and techniques. The result has been a significant step forward in our ability to interrogate atomic and electron structure at the Angstrom level. Particularly the rapid development of in-situ methods has allowed the observation of dynamic processes and the direct correlations between structure and properties. The goal of the symposium is to bring together and stimulate discussion among researchers from various disciplines (physics, chemistry, materials science, mineralogy) who develop and apply advanced TEM techniques to studying and understanding materials.
A Joint session with division "Microprobes", MI, takes place on Monday morning from 10:15 to 13:15 in H4 within this Topical session.

Topical session "Combinatorial Materials Science"

Organizers: Prof. Dr. Jörg Neugebauer (MPIE Düsseldorf), Prof. Dr. Ralf Drautz (Ruhr Universität Bochum), Prof. Dr. Jochen Schneider (RWTH Aachen)

In this symposium we address the discovery and optimization of materials through high-throughput experimentation. Suggested topics for contributions are: combinatorial synthesis of thin film and bulk materials libraries, high-throughput characterization of materials, up-scaling from combinatorial data to novel materials.

Topical session "Quasicrystals and Complex Metallic Alloys"

Organizer: Prof. Dr. Hans-Rainer Trebin (Universität Stuttgart)

Invited talks of the joint symposium SYTS (DF, DS, HL, MA, MI, MM, TT) "Thermoelectric and Spincaloric Transport in Nanostructures"

See SYTS for the full program of the symposium.

SYTS 1.1	Wed	9:30–10:00	H1	**Transport in Old and New Thermoelectric Materials** — •David Singh
SYTS 1.2	Wed	10:00–10:30	H1	**Binary oxide structures as model systems for thermoelectric transport** — •Peter J. Klar, Christian Heiliger
SYTS 1.3	Wed	10:30–11:00	H1	**Functional oxides films: from single crystals to polycrystalline substrates** — •Wilfrid Prellier
SYTS 1.4	Wed	11:00–11:30	H1	**The Planar Nernst Effect and the Search for Thermal Spin Currents in Ferromagnetic Metals** — •Barry Zink
SYTS 1.5	Wed	11:30–12:00	H1	**Tunneling magneto thermopower in magnetic tunnel junction nanopillars** — Niklas Liebing, Santiago Serrano-Guisan, Patryk Krzysteczko, Karsten Rott, Günter Reiss, Jürgen Langer, Berthold Ocker, •Hans Werner Schumacher

Invited talks of the joint symposium SYMM (BP, CPP, DY, MM) "Computational Challenges in Scale-Bridging Modeling of Materials"

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:00	H1	**Challenges for first-principles based computation of properties of oxide materials** — •Karsten Albe
SYMM 1.2	Thu	10:00–10:30	H1	**Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales** — •Peter Gumbsch, Matous Mrovec, Kinshuk Srivastava, Daniel Weygand
SYMM 1.3	Thu	10:30–11:00	H1	**Crucial Issues and Future Directions of Through-Process Modeling** — •Guenter Gottstein
SYMM 1.4	Thu	11:00–11:30	H1	**Adaptive Resolution Simulations for Soft Matter: Applications and New Developments** — •Kurt Kremer
SYMM 1.5	Thu	11:30–12:00	H1	**Materials by design** — •Markus Buehler

Invited talks of the joint symposium SYES (O, DS, HL, MA, MM, TT) "Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials"

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello
SYES 1.2	Fri	10:00–10:30	H1	**Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl
SYES 1.3	Fri	10:30–11:00	H1	**Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan
SYES 1.4	Fri	11:00–11:30	H1	**New ferroelectrics and antiferroelectrics by design** — •Karin Rabe
SYES 1.5	Fri	11:30–12:00	H1	**The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:30–20:30 H24

This year's general meeting of the Metal and Materials Physics Division (FV MM) is taking place on Wednesday at 19:30 in room H24 after the invited talks (Hauptvorträge) by S. Roberts and R. Bennewitz and the following social gathering. The meeting will be opened with a short welcome address and the report of the chairman of the Metal and Materials Physics Division (AGMM). Afterwards, all attendees are invited to elect a new Chairman of the "Fachverband Metall- und Materialphysik" and to suggest symposia and speakers which could be invited for the next spring meeting in Dresden, 30th March to 04th April 2014. Everybody is highly welcome to join the social gathering and participate at the annual meeting directly afterwards.

MM 1: Invited Talk (Hauptvortrag): Dunin-Borkowski

Time: Monday 9:30–10:00 Location: H24

Invited Talk MM 1.1 Mon 9:30 H24

New opportunities and challenges in chromatic aberration corrected and in situ transmission electron microscopy — •Rafal E. Dunin-Borkowski[1], Lothar Houben[1], Juri Barthel[1], Andreas Thust[1], Chris Boothroyd[1], Martina Luysberg[1], Andras Kovacs[1], Martial Duchamp[1], and Joachim Mayer[2] — [1]Forshungszentrum Jülich, Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany

In the most recent generation of transmission electron microscopes, chromatic aberration correction promises to provide improved spatial resolution and interpretability when compared with the use of spherical aberration correction alone, especially at lower accelerating voltages. The reduced dependence of image resolution on energy spread offers benefits for conventional bright-field and dark-field imaging, less refocusing is necessary between regions of different specimen thickness, large energy windows and large objective aperture sizes can be used in energy-filtered transmission electron microscopy, and a spatial resolution of better than 0.5 nm can be achieved with the conventional microscope objective lens switched off. In this talk I will present a selection of initial calibrations and test results obtained in both high-resolution and Lorentz modes from a recently installed transmission electron microscope equipped with a combined spherical and chromatic aberration corrector on the objective lens. These developments and results will be discussed in the context of in situ experiments, including the use of microscopes that are equipped with larger pole-piece gaps.

MM 2: Topical Session: TEM-Symposium - Joint Session with MI I

Time: Monday 10:15–11:30 Location: H4

Topical Talk MM 2.1 Mon 10:15 H4

The potential of valence electron energy-loss spectroscopy to probe local optical properties and band structure information in scanning transmission electron microscopy — •Rolf Erni — Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Valence electron energy-loss spectroscopy (VEELS) in scanning transmission electron microscopy (STEM) offers the possibility to measure band structure information and in particular band gap and transition energies of materials with (sub-)nanometer spatial resolution. Although the technique has been used to reliably identify dielectric information of various bulk and nanomaterials, VEEL spectra contain a wealth of spectral contributions which can complicate the extraction of the desired information. Retardation effects, such as Cerenkov losses, or the excitation of guided light modes as well as surface and finite-size effects can alter the bulk dielectric function contained in VEEL spectra. The dielectric theory describing these effects has been known for a long time, but the incorporation of these effects into routine simulations has not yet become standard. For materials of known dielectric function, it is possible to analyze the origin of individual spectral signatures. This allows for predicting possible spurious effects of unknown materials. The present contribution provides an overview of the applicability of VEELS for the study of nanomaterials, interface and surface effects, combining experiments with simulations which are adequate to address spectral signatures that are not describable by the common energy-loss function of bulk materials.

Topical Talk MM 2.2 Mon 10:45 H4

Application of Electron Energy-Loss Spectroscopy to Study Nanostructures and Interfaces — •Christina Scheu — Department of Chemistry & Center for NanoScience, Ludwig-Maximilians-University of Munich, 81377 Munich, Germany

Electron energy-loss spectroscopy (EELS) in the transmission electron microscope (TEM) provides information on the optical properties, the chemical composition and the electronic structure of materials down to the nanometer regime or even below. These informations are obtained by analyzing the spectral features occurring in the low-loss region (up to energy-losses of around 50 eV) or with the help of the element-specific ionization edges which are found in the core-loss region (above 50 eV). In this talk the different features are discussed under the impact of possible interface and nanostructure investigations. It will be shown that the band gap of individual semiconducting oxide nanosheets can be obtained by comparing experimental data acquired with a monochromated TEM to density functional theory calculations. Furthermore, electronic structure changes occurring at strained oxide-oxide interface will be presented. These changes can be investigated by analyzing the electron energy-loss near-edge structure which is associated with each element-specific ionization edge and which contains information on e.g. bonding characteristics and nominal oxidation states of the probed interfacial atoms.

MM 2.3 Mon 11:15 H4

Effect of lens aberrations on strain measurements from Convergent Beam Electron Diffraction patterns — •Christoph Mahr[1], Knut Müller[1], Andreas Rosenauer[1], Marco Schowalter[1], Daniel Erben[1], Josef Zweck[2], and Pavel Potapov[3] — [1]Universität Bremen — [2]Universität Regensburg — [3]GlobalFoundries, Dresden

This presentation deals with the effect of lens aberrations in a transmission electron microscope (TEM) on strain measurements in semiconductor heterostructures using Strain Analysis by Nano-Beam Electron Diffraction (SANBED). As this method is based on the analysis of disc positions in a series of Convergent Beam Electron Diffraction (CBED) patterns, strain measurements could be inexact e.g. due to lens aberrations of the projection system. The distortion field is detected by comparing the disc positions in an experimental CBED pattern obtained from a substrate region of the specimen with theoretical ones. Based on this field, we show how the distortions in all CBED patterns of a series can be corrected. Subsequently the effect of the correction on the strain measurements is investigated. It is found that the averaged difference between strain from uncorrected patterns and strain from corrected patterns is in the order of 10^{-3} %. This difference is one order less than the precisions of contemporary strain measurement techniques, such as SANBED, which has a precision of $(7-9)\cdot 10^{-2}$ %. Consequently, the effect of distortions in a diffraction pattern can be neglected at the moment. The effect could become more evident, when the precision of strain measurements is improved.

MM 3: Computational Materials Modelling - Fundamentals

Time: Monday 10:15–11:30 Location: H24

MM 3.1 Mon 10:15 H24

New developments in non-local density functional theory — •Riccardi Sabatini[1,2] and Stefano de Gironcoli[2] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH) — [2]Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy

Van-der-Waals dispersive interactions are an essential component in the description of soft matter and in many other systems, from metal adsorbates to hydrophobic and hydrophilic interactions. In the last years a great effort has been made within the framework of density-functional theory to overcome the limitations of local or semi-local functionals, and a new class of non-local functionals is now able to

take into account dispersive interacitons. We present some of our recent contributions to this field, and some selected applications. In particular, i) we developed and implemented in the Quantum-ESPRESSO distribution a new functional, inspired by the work of Vydrov and Van Voorhis [PRL 103, 06300], that can work very efficiently in a plane-wave basis and shows excellent performance on the reference set S22 of non-covalent complexes, ii) we extended and implemented in density-functional perturbation theory the formalism to treat non-local functionals of the form suggested by Dion et al. [PRL 92, 246401 (2004)], obtaining a simple and efficient way to calculate the vibrational properties of soft materials from first-principles. Finally, we present results on graphite and simple molecules, where these new tools are benchmarked and compared with experimental results or other theoretical approaches.

MM 3.2 Mon 10:30 H24

The physical solution of the *GW* approximation — •Falk Tandetzky, Kay Dewhurst, Sangeeta Sharma, and E.K.U. Gross — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We show[1] that the equations underlying the *GW* approximation have a large number of solutions. To the best of our knowledge no such extra solutions have been reported in the literature yet. This raises the questions: Which is the physical solution? And why do numerical methods converge to it, rather than to one of the spurious solutions? We provide theorems which answer both of these questions. These theorems are general enough to cover a large class of similar algorithms. This fact is important for understanding how vertex corrections can be treated without running into unphysical solutions.

[1] F. Tandetzky, J. K. Dewhurst, S. Sharma, E. K. U. Gross: arXiv:1205.4274

MM 3.3 Mon 10:45 H24

How van der Waals Interactions Influence Cohesive Properties of Solids — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Standard semilocal and hybrid density functionals are widely used for studying cohesive properties of many covalent, metallic, and ionic materials. Only recently it has been recognized that long-range van der Waals (vdW) interactions, that are missing in all semilocal and hybrid functionals, are important for an accurate description of cohesion in solids. Here we construct a database of 64 solids where reference cohesive properties are obtained from a critical revision of the available experimental data. All-electron DFT calculations with explicit treatment of zero-point vibrations for all cohesive properties are carried out using the local-density approximation (LDA), Perdew-Burke-Ernzerhof (PBE) GGA, and the empirical meta-GGA M06-L [1] functionals. For 23 semiconductor solids, we also carry out PBE and M06-L calculations with the inclusion of fully screened long-range vdW energy [2]. We find that PBE is the most systematic from the three employed functionals, and its accuracy is improved by a factor of two after the inclusion of vdW interactions. The LDA functional considerably overbinds for all the studied solids. The M06-L functional describes middle-range correlation better for certain semiconductors and ionic crystals, but fails for heavier semiconductors and metals. [1] Zhao and Truhlar, JCP (2006). [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

MM 3.4 Mon 11:00 H24

The importance of many-body dispersion interactions for molecular materials — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

It is now well established that dispersion interactions are essential to the stability and properties of soft-matter and molecular materials. However, many computational approaches use simple pairwise approximations to include these interactions, ignoring their origin in collective many-body plasmonic excitations. Using the recently developed many-body dispersion (MBD) method (PRL 108, 236402; PNAS 109, 14791) and a database of molecular-crystal structures, we show that a realistic many-body treatment of dispersion interactions has a significant impact on molecular-crystal stability. Crucially, coupling the MBD method with DFT calculations allows *ab initio* modelling to reach within the highly coveted "chemical accuracy" with respect to experimental enthalpies of sublimation. The results show that the accurate modelling and prediction of molecular materials necessitates an accurate and "beyond pairwise" treatment for dispersion interactions.

MM 3.5 Mon 11:15 H24

Metamaterials and cosmological inflation — •Grigoris Panotopoulos and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

Inflation is widely accepted to be the best paradigm we have today for the physics of the early universe. It solves the lond-standing problems of hot big-bang cosmology, and at the same time it generates the primordial fluctuations responsible for the structures we observe in the universe today. On the other hand, metamaterials are laboratory made, artificial materials with new exotic properties not found in other substances in nature, and they can have numerous interesting applications. In the present work we make a connection between hyberbolic metamaterials and cosmological inflation. We show that if the permittivities of the metamaterial are appropriately chosen, then the Maxwell's equation for the light propagation in the sample matches the equation for the metric perturbation, and for a concrete inflationary model we find exact analytical solutions. Therefore, not only can inflation be reproduced in the laboratories, which is interesting on its own, especially now that the Planck mission is taking data and may see gravitational waves as predicted from inflation, we may also obtain interesting solutions for the electric field in the metamaterial (Bessel functions), based upon cosmological solutions.

MM 4: Topical Session: Quasicrystals & Complex Metallic Alloys I

Time: Monday 10:15–11:30 Location: H25

Topical Talk MM 4.1 Mon 10:15 H25

Observation of kinks and antikinks in colloidal monolayers driven across periodic and quasiperiodic surfaces — •Clemens Bechinger — Universität Stuttgart, 2. Physikalisches Institut, Stuttgart

Friction between solids is responsible for many phenomena like earthquakes, wear or crack propagation. Unlike macroscopic objects which only touch locally due to their surface roughness, spatially extended contacts form between atomically flat surfaces. They are described by the Frenkel-Kontorova model which considers a monolayer of interacting particles on a periodic substrate potential. In addition to the well-known slip-stick motion such models also predict the formation of kinks and antikinks which largely reduce the friction between the monolayer and the substrate. Here, we report the direct observation of kinks and antikinks in a two-dimensional colloidal crystal which is driven across different types of ordered substrates [1]. We show that the frictional properties only depend on the number and density of such excitations which propagate through the monolayer along the direction of the applied force. In addition, we also observe kinks on quasicrystalline surfaces which demonstrates that they are not limited to periodic substrates but also occur under more general conditions.

[1] T. Bohlein, J. Mikhael, and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, Nature Materials 11, 126 (2012).

MM 4.2 Mon 10:45 H25

Geometric Properties of *N*-fold Symmetric Quasicrystals — •Johannes Roth — ITAP, Universität Stuttgart

Rhombic quasicrystals with n-fold planar symmetry contain configurations with $2n$- or n-fold point symmetry. These "flowers" or "stars" are very predominant in fivefold quasicrystals and play an important role for example in the stabilization of colloidal quasicrystals. We have determined the number of stars directly up to n=11. We observe that if n increases, the number of stars decreases more than exponentially. Thus we argue that finite tiling patches with very high n up to 30, which many groups study experimentally, should not be called "quasicrystals" since these patches do not form representative samples of a quasicrystal due to the small sample size.

Laser potentials which are generated by the superposition of har-

monic waves exhibit local isomorphism classes much like rhombus tilings. While these classes are well known for tilings, we describe them for n-fold symmetric laser fields using the methods of Mermin et al. and show how many free parameters exist.

Topical Talk MM 4.3 Mon 11:00 H25

Recent advances in mathematical diffraction theory — •Uwe Grimm — Department of Mathematics and Statistics, The Open University, Walton Hall, Milton Keynes MK7 6AA, UK

The discovery of quasicrystals called for an extension of classical diffraction results to aperiodic systems. For cut and project sets, it was shown that the diffraction is pure point, and the locations and intensities of Bragg peaks can be calculated explicitly. More recently, rigorous and constructive approaches to the case of diffuse scattering have led to a better understanding of systems with singular continuous and absolutely continuous diffraction. This talk reviews the development of mathematical diffraction theory following the discovery of quasicrystals.

MM 5: Functional Materials - Battery Materials I

Time: Monday 10:15–11:30 Location: H26

MM 5.1 Mon 10:15 H26

Charge Transfer Reactions at Electrode Materials for Lithium Ion Batteries — •Fabian Wunde, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Universität Münster

Powerful Lithium Ion Batteries on the one hand have to provide high energy densities, and on the other hand this energy has to be available in short period of time, i.e. they have to be capable of high charge/discharge rates. In general, these high charge/discharge rates result in both, a capacity loss and in large overpotentials. Since the hopping rate of lithium atoms, which are passing the interface between the electrode and the ion conductor, is determined by an activation energy, an external overpotential will increase the number of successful lithium transitions. In our work we studied in detail the overpotentials of ion-beam-sputtered LiFePO4 thin films, which serve as a model system. By the use of cyclic voltammetry, a linear relationship between the scan rate and the measured overpotential is observed. Solving the Butler-Vollmer equation under linear sweep boundary conditions confirms this linear behavior and finally allows us to measure the hopping rate of lithium in case of LiFePO4.

MM 5.2 Mon 10:30 H26

First-principles study of multilayer graphynes for lithium ion battery anodes — •Hoonkyung Lee — 1Division of Quantum Phases & Devices, School of Physics, Konkuk University, Seoul 143-701, South Korea

Graphynes, two-dimensional layers of sp- and sp2-bonded carbon atoms, have recently received considerable attention because of their potential as new Dirac materials. Here, focusing on their large surface area, we explore the applicability of graphynes as lithium ion battery anodes through the first-principles density functional calculations. We have found that Li potential energies are in the range suitable to be used as anodes. Furthermore, the maximum composite of Li-intercalated multilayer α- and γ-graphynes is found to be C6Li3, which corresponds to a specific capacity of 1117 mAh g-1, twice as large as the previous theoretical prediction for graphynes. The volumetric capacity of Li-intercalated multilayer α- and γ-graphynes is 1364 and 1589 mAh cm-3, respectively. Both specific and volumetric capacities of Li-intercalated graphynes are significantly larger than the corresponding value of graphite, from which we conclude that multilayer graphynes can serve as high-capacity lithium ion battery anodes.

MM 5.3 Mon 10:45 H26

Morphology and size control of LiMnPO4 nano- and microcrystals — •Christoph Neef[1], Carsten Jähne[1], Hans-Peter Meyer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, D-69120 Heidelberg, Germany — [2]Institut für Geowissenschaften, University of Heidelberg, D-69120 Heidelberg, Germany

A microwave-assisted hydrothermal synthesis route was applied to grow LiMnPO4 micro- and nanocrystals, starting from acetate precursors. The crystal size can be manipulated over a range of two orders of magnitude (from around 10 um down to a few 100 nm) by appropriate adjustment of both synthesis conditions: the precursor concentration and the pH-value of the reactant. The resulting crystal morphology as well as the materials texture and agglomeration tendency were investigated by means of XRD and SEM. The influence of morphology, size, and agglomeration on the electrochemical properties were investigated by cyclic voltammetry. Reversible electrochemical activity appears at particle size below 1 um.

MM 5.4 Mon 11:00 H26

Lithium Ion Transport in LCO-Li-SiO2 multilayer stacks — •Frank Berkemeier, Tobais Stockhoff, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm Str. 10, D-48149 Münster

Thin films of lithium cobalt oxide (LCO) and lithium silicate glass are prepared by ion beam sputter deposition. The capability of the LCO films to reversibly store and release lithium ions is proven by means of cyclic voltammetry and chronopotentiometry, while the ionic conductivity of the silicate glass is measured by electrochemical impedance spectroscopy. Furthermore, by measuring the correlation between the transmission of visible light through the LCO films and their lithium content, the intercalation/deintercalation process is studied in detail by optical transmission measurements. Applying these transmission measurements in case of LCO films of different thickness between 10 and 500 nm, allows us to determine the interface barriers for the transfer of lithium ions from the liquid electrolyte into LCO. By depositing an additional layer of silicate glass onto the LCO film, the transmission measurements are also used to obtain quantitative information about the mobility of lithium ions within the glass film.

MM 5.5 Mon 11:15 H26

Thin film batteries based on LiPON thin films — •Susann Nowak, Frank Berkemeier, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the preparation of a complete thin film solid state lithium-ion battery by depositing a LiPON (lithium phosphorus oxynitride, $Li_3N_x(PO_4)_{1-x}$) layer between two metallic thin film electrodes on silicon. It is shown that during the first cycle of cyclic voltammetry measurements, electrochemically active interface regions are formed, serving as anode and cathode, respectively, and thus the layer stack acts as a complete electrochemical thin-film cell. These cells are investigated by means of temperature-dependent electrochemical impedance spectroscopy (EIS) and transmission electron microscopy (TEM), with special emphasis on the reactive layer between metallic electrode and LiPON. A whole typical battery (excluding the substrate) is just about 700 nm thick. To achieve such a thin geometry very smooth layer surfaces are necessary, which are prepared by reactive ion-beam sputtering of Li_3PO_4, using argon as sputter gas and nitrogen as reactive additive.

Due to their well-defined geometry, these samples are well suited to study interface reactions, with the aim to further improve lithium-ion batteries.

MM 6: Topical Session: TEM-Symposium - Joint Session with MI II

Time: Monday 11:45–13:15 Location: H4

Invited Talk MM 6.1 Mon 11:45 H4

Prospects for mapping spins with atomic resolution in TEM — •Johan Verbeeck — EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

In this talk, the prospects for mapping spins with atomic resolution in a TEM will be outlined. The proposed method is based on the use of electron vortex STEM probes. Such probes contain a helical phase of the type $\psi(r,\phi) = f(r)e^{im\phi}$ with m the so-called topological charge. This topological charge is responsible for an orbital angular momentum of $m\hbar$ and a magnetic moment of $m\mu_B$ carried by the electron probe. The phase symmetry affects the dipole selection rules in inelastic scattering which allows us to measure the change in magnetic quantum number upon excitation. As vortex electron probes can now be made to atomic size, we also expect to get magnetic information from individual atom columns in atomic resolution STEM-EELS experiment. Indeed, simulations show that even for thicker samples where multiple scattering can become important, an atomic resolution signal remains that contains information on the spin and orbital magnetic moment of a targeted atom with atomic resolution. Preliminary experiments are shown and the different experimental obstacles will be discussed.

Invited Talk MM 6.2 Mon 12:15 H4

Structural Characterization of nc-Si / SiO_x based quantum superstructures for the solar cell application by aberration-corrected high resolution electron microscopy — •Maryam Beig Mohamadi[1], Birger Berghoff[2], and Joachim Mayer[1,3] — [1]Central Facility for Electron Microscopy, RWTH Aachen, Ahornstrasse 55, 52074 Aachen, Germany — [2]Institute of Semiconductor Electronics, RWTH Aachen University, Sommerfeldstr.24, 52074 Aachen, Germany — [3]Peter Gruenberg Institute and Ernst Ruska Center for Microscopy and Spectroscopy with Electrons, Research Centre Jülich, D-52425 Jülich, Germany

In the frame of SINOVA project, two nano-structured systems were investigated, a-Si/SiO_x and SiO_x/SiO_2 multilayer systems. After annealing the sample, Si nano-crystals formed within an amorphous SiO_2 matrix. The morphology and distribution of the nc-Si precipitates within the amorphous layer, their nucleation and growth kinetics, the thickness of conducting layers and the diffusion of O or Si through interfaces were analyzed by high resolution transmission electron microscopy, energy filtered transmission electron microscopy and electron energy loss spectroscopy. We employed aberration-corrected TEM microscopes to reveal the crystalline structure and the chemical distribution of Si on the atomic scale. It is observed that the mean size of the QDs and their distribution in the dielectric matrix changes by the initial thickness of the SiO_x layer. The kinetics of the formation of nc-Si precipitates in Si-rich layers sandwiched between barrier layers was studied as a function of stacking period and oxygen content in the system.

MM 6.3 Mon 12:45 H4

Aktuelle Ergebnisse mit den HRTEM JEOL JEM-ARM 200F — •Jürgen Heindl — JEOL (Germany) GmbH; Oskar-von-Miller-Str. 1a; 85386 Eching; Germany

Das JEOL JEM-ARM 200F ist das erste Transmissions-Elektronen-Mikroskop das von Grund auf ausschließlich für den Betrieb mit Korrektoren für die Aberration der Linsen entwickelt wurde. Es können sowohl die limitierenden Aberrationen im STEM (Scanning Transmission Electron Microscopy) Betrieb (CESCOR) als auch die des Objektivs in der hochauflösenden Transmissionselektronenmikroskopie (HREM, CETCOR) bzw. beide ausgeglichen werden. Ergänzend kann das System an Stelle der Schottky-Feldemissionskathode mit einer völlig neuartigen kalten Feldemissionsquelle (ColdFEG) mit sehr geringer Energiebreite mit hoher Intensität ausgerüstet werden. Im STEM-Betrieb zeigt die ColdFEG deutlich verbesserte Abbildungsleistungen gegenüber einer Schottky-Quelle, was bei der direkten Abbildung der H-Atome in Yttriumhydrid gezeigt wird. Im HREM-Betrieb ist die ColdFEG anderen Lösungen überlegen, weil die geringe Energiebreite der Primärelektronen unmittelbar auf die Auflösung verbessert. Der Nachteil einer polychromen Beleuchtung entfällt; die Bildergebnisse sind vollumfänglich simulierbar. Ein vollanalytisches JEM-ARM200F zeichnet sich durch den neuen JEOL Centurio-EDX- Detektor aus. Der Centurio-Detektor erreicht seine sehr hohe Empfindlichkeit durch eine aktive Fläche von 100 mm2 und einen Raumwinkel von 1 sr. Mit der neuen ColdFEG wird ein Echtzeit-EDX-Mapping an SrTi03 und GaAs gezeigt.

MM 6.4 Mon 13:00 H4

Investigation of innovative capacitors for energy storage based on 0-3 composites — •Jens Glenneberg, Gerald Wagner, Alexandra Buchsteiner, Mandy Zenkner, Thomas Grossmann, Claudia Ehrhardt, Stefan G. Ebbinghaus, Martin Diestelhorst, Sebastian Lemm, Wolfram Münchgesang, Horst Beige, and Hartmut S. Leipner — Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle

Currently energy storage is an interesting and important topic. Next to accumulators, thin film capacitors with high energy densities are feasible. The aim of our work is to develop novel capacitors exhibiting several advantages like very quick charging and discharging times, long lifetimes and high robustness as well as low manufacturing costs.

For this purpose, ceramic nanoparticles with perovskite structure and high permittivities ($BaTiO_3$, $Ba(Ti,Ge)O_3$, $CaCu_3Ti_4O_{12}$) are embedded in either an organic polymer or an inorganic glass matrix. In order to achieve a uniform dispersion, the nanoparticles are coated with a specific surfactant depending on the matrix. Size and distribution of the embedded particles have a strong effect on the electrical properties of the capacitor dielectrics. Therefore, accurate knowledge of the microstructure is necessary. The single composites are imaged via environmental scanning electron microscopy (ESEM) in secondary electron (SE) and backscattered electron contrast (BSE). Additionally, transmission electron microscopy (TEM) investigations are carried out and energy-dispersive X-ray spectroscopy is conducted in order to get compositional information.

MM 7: Computational Materials Modelling - Methods

Time: Monday 11:45–13:00 Location: H24

MM 7.1 Mon 11:45 H24

Quantum electrodynamics of nanostructures — •Walter Tarantino, J. K. Dewhurst, S. Sharma, and E. K. U. Gross — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

The project is aimed to develop a time-dependent functional theory for quantum electrodynamics. We want to establish a Kohn-Sham system for relativistic electrons, as well as positrons and photons. Apart from representing the natural generalization of the usual non-relativistic many-body problem, the approach will provide us with a novel instrument for computational investigations of the interaction between light and matter. Details about preliminary results on KS systems and the effective (exchange-correlation) potentials will be presented.

MM 7.2 Mon 12:00 H24

An Approach to Coarse-Grained Molecular Dynamics — •David Edmunds, Paul Tangney, Dimitri Vvedensky, and Matthew Foulkes — Imperial College London, London, UK

Traditional molecular dynamics (MD) simulations provide an effective method for simulating the evolution of a system at the atomic level, without the associated computational cost of ab-initio methods such as density-functional theory. However, many physical and biological processes occur on length scales of millimetres and time scales of seconds, which remain out of reach to fully atomistic simulations on even the most powerful modern supercomputers.

Fortunately, a family of techniques known as coarse-grained molecular dynamics (CGMD) exists, which can bridge the gap between atomistic simulation and the mesoscale. These approaches allow for a larger

time step to be used, as the fast degrees of freedom in the system have effectively been integrated out. They can also produce CG potentials which are much less computationally intensive than their all-atom counterparts. This results in CG simulations which are several orders of magnitude faster than all-atom MD, allowing the simulation of billion atom systems on standard desktop computers.

We present two strategies for deriving a coarse-grained pairwise interaction potential, based on the internal energy and free energy of a pair of constrained molecules. We benchmark these methods against a fully atomistic MD simulation of interacting C60 buckyballs, chosen since they are trivially represented by a single CG site located at their centre of mass.

MM 7.3 Mon 12:15 H24

New Methods for Calculating the Free Energy of Charged Defects in Solid Electrolytes. — •Robert Horton, Andrew Haslam, Amparo Galindo, George Jackson, and Michael Finnis — Imperial College London, London, United Kingdom

Solid electrolytes are utilised in a myriad of technological applications ranging from fuel cells to gas sensors. It is the presence of charged defects in their lattice structure that is primarily responsible for their useful electrolytic behaviour [1] and, accordingly, a detailed understanding of the thermodynamic behaviour of these defects is highly desirable. Analytic models for describing the thermodynamic contribution of defects break down at concentrations of a few percent, due to the long-ranged nature of the Coulombic defect-defect interactions. We have developed and tested an alternative scheme, using Wang-Landau sampling [2], a temperature-independent Monte Carlo method, to statistically calculate the free energy of the system at the atomistic level. It is interesting to see that this calculated free energy can be fitted by traditional functional forms, such as regular-solution and Redlich-Kister, with which the thermodynamic properties of the system can be calculated.

[1] S. C. Singhal (2000). Science and Technology of Solid-Oxide Fuel Cells. MRS Bulletin, 25, pp 16-21 doi:10.1557/mrs2000.13

[2] F. Wang and D. P. Landau, (2001). Physical Review E. 64, 056101-1-16.

MM 7.4 Mon 12:30 H24

A polarizable potential for the Al_2O_3-Y_2O_3 system — •Hannes Guhl, Matthew Foulkes, Michael Finnis, and Paul Tangney — Department of Physics and Materials, Imperial College London, SW7 2AZ, UK

The high-temperature oxidation rate of alloys containing aluminium is much reduced in the presence of rare earth (RE) elements such as yttrium. Apparently, the grain boundaries acting as the primary channel via which oxygen and metal ions cross the oxide film are effectively blocked by the segregating RE elements, yet it is controversial whether or not this "reactive element effect" is due to the alteration of the electronic- or atomic structure.

We apply density functional theory (DFT) as the best available tool for addressing the subtle interplay of defect formation energies and mobilities, including yttrium in grain boundaries of alumina. However, due to their complexity, realistic structural models of grain boundaries cannot be established with DFT alone. Therefore, we present here an empirical, computationally cheap, polarizable ion potential, which matches the DFT interatomic forces in Y doped alumina. We make a direct comparison between computed and experimentally measured grain boundary structures and energies. In addition, the potential captures the essential energetic and structural properties of pure Y_2O_3 as well as of mixed phases such as $Y_3Al_5O_{12}$, suggesting that it will be useful for atomistic studies of the complex thermodynamics across the Al_2O_3-Y_2O_3 system.

MM 7.5 Mon 12:45 H24

Exploring the exohedral reactivity of endohedral metallofullerenes (EMFs): the encapsulation effect and the fullerene strain energy — •Silvia Osuna[1,2], Marc Garcia-Borràs[2], Josep M. Luis[2], Marcel Swart[2,3], and Miquel Solà[2] — [1]University of California, Los Angeles (UCLA), Los Angeles, USA — [2]Universitat de Girona, Girona, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

Endohedral metallofullerenes (EMFs) have attracted increasing attention in the last years due to their potential applications in the field of biology and medicine as a result of the magnetic, spectroscopic, and nuclear properties of the metal ions encapsulated inside. [1] The third most abundant fullerene is the trimetallic nitride template (TNT) EMF, $Sc_3N@C_{80}$. In these compounds, there exists a formal electronic transfer of six electrons from the M_3N unit to the fullerene structure ($M_3N^{+6} : C_x^{6-}$). Consequently, the metal cluster encapsulated inside has a huge influence on the reactivity of these compounds, which is, in general, reduced in TNT EMFs as compared to free fullerenes. In the present work, we perform a theoretical study of the thermodynamics and the kinetics of the [4+2] Diels-Alder (DA) reaction of s-cis-1,3-butadiene with several isomers of free fullerene cages (i.e $I_h - C_{80}$, $D_{5h} - C_{80}$, $D_{3h} - C_{78}$) and their respective TNT-EMF compounds encapsulating differently sized cluster metals (i.e. Sc_3N, Y_3N, Lu_3N, Gd_3N, Ti_2C_2). (1) Osuna, S. et al. Phys. Chem. Chem. Phys. 2011, 48, 2486-2488.

MM 8: Topical Session: Quasicrystals & Complex Metallic Alloys II

Time: Monday 11:45–13:00 Location: H25

MM 8.1 Mon 11:45 H25

Electronic Wave Functions of Quasiperiodic Systems in Momentum Space — •Stefanie Thiem, Sebastian Rolof, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

In quasicrystalline tilings often multifractal electronic wave functions can be found, which are neither extended over the whole system nor exponentially localized. In order to obtain a better insight into their localization properties, we study the wave functions of quasiperiodic tilings in momentum space. The models are based on one-dimensional quasiperiodic chains, in which the atoms are coupled by weak and strong bonds aligned according to the Fibonacci sequences. The associated hypercubic tilings and labyrinth tilings in d dimensions are then constructed from the direct product of d such chains.

The results show that each wave function is described by a hierarchy of wave vectors and is always dominated by a single wave vector which is directly related to the energy eigenvalue of the wave function. Combining the information of all wave functions of the system, we observe a hierarchy of branches with different intensities. Each branch is a copy of the main branch containing the dominant wave vectors for each wave function. Using perturbation theory and a renormalization group approach we determine the shape of the branches for the limit cases of weak and strong coupling.

MM 8.2 Mon 12:00 H25

Confirmation of the Random Tiling Hypothesis for a Decagonal Quasicrystal — •Alexander Kiselev[1], Michael Engel[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Department of Chemical Engineering, University of Michigan, USA

The random tiling hypothesis of Henley and Elser states, that the configurational entropy due to the phason flips stabilizes a quasicrystal at elevated temperatures and leads to a periodic crystal at low temperatures. Here, we study the role of entropy for a monatomic two-dimensional decagonal model quasicrystal, whose atoms interact by a double-well Lennard-Jones-Gauss pair potential. We calculate the free energy of the system, which can be split up into a phonon part and a configurational part. The phonon part of the free energy is calculated with molecular dynamics using the Frenkel-Ladd method. For the configurational part a new Ising-type model of uncorrelated flips is employed in Monte Carlo simulations. We observe that the free energy takes a square-gradient form of the phason displacement as predicted by the random tiling hypothesis and determine phason elastic constants over a large range of temperatures. The free energy calculations confirm a phase transition from an entropically stabilized decagonal random tiling phase to an energetically stabilized periodic crystal. Thus, for the first time, a virtual quasicrystal confirms all predictions of the random tiling hypothesis in a fully atomistic model [1].

[1] A. Kiselev, M. Engel and H.-R. Trebin, arXiv:**1210.4227** (2012)

Topical Talk MM 8.3 Mon 12:15 H25

Self-assembly and packing of polyhedra into complex crystal structures — •Michael Engel[1], Pablo F. Damasceno[1], Amir Haji-Akbari[2], and Sharon C. Glotzer[1] — [1]Chemical Engineering, University of Michigan, USA — [2]Chemical and Biological Engineering, Princeton University, USA

Isolating the role of building block shape for self-assembly and packing provides insight into the ordering of molecules and the crystallization of colloids, nanoparticles, proteins, and viruses. We investigated a large group of polyhedra whose phase behavior arises solely from their anisotropic shape by exploiting entropic driving forces. Our results demonstrate a remarkably high propensity for thermodynamic self-assembly and structural diversity [1]. In particular, I will discuss the formation and geometric stabilization of a dodecagonal quasicrystal with tetrahedra [2] as well as the appearance of topologically close-packed phases. All of the crystal structures we observe have analogues in the elements and can be understood by relating shape to atomic interactions. It turns out that the structural complexity is particularly high, when entropy and geometric constraints compete with locally dense configurations.

[1] P.F. Damasceno et al. Science 337, 453 (2012)
[2] A. Haji-Akbari et al. Nature 462, 773 (2009)

MM 8.4 Mon 12:45 H25

Symmetry and Chemistry of Complex Intermetallics — •Julia Dshemuchadse and Walter Steurer — Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

Complex intermetallic structures can be found in many different systems and exhibit giant unit cells. They feature a number of peculiar properties, but until recently, no unifying approach has been applied to describe their structures. To achieve a deeper understanding of their building principles, we are examining the structures of complex intermetallics on three different levels. For a generalized definition, we are statistically comparing the distribution of complex intermetallics over the entirety of intermetallic structures. Secondly, we have picked out highly symmetric lattices (*e.g.*, [1]), which feature a large number of complex structures, and analyze the distribution of different structure types within these groups, as well as their interrelations. The third step focuses on specific intermetallic systems featuring multiple complex compounds and describes their special geometries in a comparative way to reveal similarities and distinctions.

By trying to better understand complex intermetallic structures, we hope to be able to gain more profound knowledge on the formation of metallic matter in general.

[1] J. Dshemuchadse, D. Y. Jung, W. Steurer, Acta Cryst. B67, 269-292 (2011).

MM 9: Functional Materials - Battery Materials II

Time: Monday 11:45–13:00 Location: H26

MM 9.1 Mon 11:45 H26

New Approach to Deposit Functional Thin-Films for Battery Application: CO2-Laser Assisted Chemical Vapor Deposition — •Christoph Loho[1,2], Azad Darbandi[1,2], Ruzica Djenadic[1,2,3], and Horst Hahn[1,2,3] — [1]Joint Research Laboratory Nanomaterials, Technical University of Darmstadt and Karlsruhe Institute of Technology, Germany — [2]Institute for Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Helmholtz Institute Ulm, Germany

The research on thin-film batteries is driven by an increasing demand for micro-sized power sources, because of the progressive miniaturization of electronic components over the last decades. Especially an all-solid-state thin-film battery is desirable, since its excellent safety properties and easy integration in microelectronics, e.g. in RFID tags, are outstanding advantages.

In this presentation we report on a new established technique to deposit functional thin-films for battery application. This CO2-laser assisted chemical vapor deposition (LACVD) makes use of solid precursors, which evaporate instantaneously by absorption of microwave laser radiation. The deposition of the thin-films, acting as cathode, anode or solid-state electrolyte, then takes place on a diode laser heated substrate. By tuning the process parameters several structural features, such as the degree of crystallinity, density and thickness of the films can be adjusted. As one prominent example, a thin film of LiCoO2 was deposited onto a platinum substrate and electrochemically characterized. Further investigations comprise X-ray diffraction (XRD), Raman spectroscopy as well as scanning electron microscopy (SEM).

MM 9.2 Mon 12:00 H26

Comparative computational study of Si, Ge, and Sn as anode materials for Mg batteries — •Sergei Manzhos[1], Oleksandr Malyi[2], and Teck L. Tan[2] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, Singapore 117576 — [2]Institute of High Performance Computing, A*STAR, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

Magnesium batteries are emerging as a viable high energy density alternative to Li batteries that also circumvent potential Li supply risks. Most research has focused on the design of cathode materials for Mg batteries. Mg metal, while being safer than metallic Li, results in poor reversibility. The rechargeability and voltage could be improved by using an insertion anode, but theoretical studies of high-capacity Mg insertion anodes are lacking. We present ab initio calculations of the behavior of Mg atoms in bulk Ge, Si, Sn and their Mg alloys and evaluate their potential as insertion type anode materials. We show that despite the fact that Si and Ge could provide the highest specific capacities (3817 mAh g-1 and 1476 mAh/g, respectively) for Mg storage, they result in significant lattice expansions and slow Mg diffusion. Sn appears as a more attractive anode material with the barrier to diffusion as low as 0.32 eV and the smallest expansion among the three materials.

MM 9.3 Mon 12:15 H26

A room-temperature sodium/oxygen battery — •Pascal Hartmann[1], Conrad L. Bender[1], Anna Katharina Dürr[2], Jürgen Janek[1], and Philipp Adelhelm[1] — [1]Institute of Physical Chemistry, Justus-Liebig-University Gießen, Gießen, Germany — [2]BASF SE, BCI/E-M311, Ludwigshafen, Germany

In this work we discuss the charge/discharge characteristics of analog sodium/oxygen and lithium/oxygen cells that are built up by a metallic anode, liquid electrolyte, and a porous carbon cathode. Compared to the Li/O_2 cell, the Na/O_2 cell shows a superior performance, with a higher discharge capacity at higher current densities and in addition with significantly lower overpotential for the charging process. In addition to pure oxygen, the cells were also cycled under different gas mixtures. In addition to the electrochemical measurements, we characterized the discharge products cells using x-ray powder diffraction, Raman spectroscopy, x-ray photoelectron spectroscopy, and electron microscopy. We clarified the cell reactions and the origin for the high discrepancy in the electrochemical performance for lithium and sodium based oxygen batteries. In summary, we show that the charge/discharge characteristics in analog Li/O_2 and Na/O_2 batteries significantly differ from each other: In particular the sodium based cells show higher discharge capacities at higher current densities as well as lower overpotentials for the discharge and charge reaction.

MM 9.4 Mon 12:30 H26

Electrochemical investigation and analytical TEM on sputter deposited V_2O_5 thin film electrodes — •Tobias Gallasch, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Thin film electrodes (10 nm - 200 nm) of Vanadium Pentoxide (V_2O_5) are prepared by ion beam sputtering. Cyclic voltammetry as well as chrono-potentiometric measurements demonstrate that the films reach the theoretical capacity for lithium storage of 400 mAh/g and that they can be operated in a wide current range (charge/discharge rates between C/44 and 77 C). Furthermore, the Li^+ diffusion coefficient is determined by cyclic voltammetry and compared to results of the concentration dependent GITT technique.

In contrast to electrochemical studies on bulk material, the sputter-deposited thin films of this work provide a well-defined geometry. Therefore, fundamental processes, such as Li transport and cyclic aging

can be studied in detail via analytical TEM an HR-TEM. Additionally, in this work, we are in particular studying the charge/discharge process via the EELS technique, which is sensitive on smallest changes in composition and can help to locally determine the lithium concentration within the V_2O_5 thin films.

Thus, we present a combination of fundamental electrochemical methods with high resolution and analytical TEM, to obtain detailed information about structural changes within the electrode material during the intercalation and deintercalation reaction.

MM 9.5 Mon 12:45 H26

Large Area Ultrathin Alumina Membranes to Fabricate Highly Ordered heterojunction Core-Shell Nanostructure — •Ahmed Al-Haddad[1,2], Huaping Zhao[1], Ranjith Vellacheri[1], Yan Mi[1], Samar Tarisch[1,2], and Yong Lei[1] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, University of Al-Mustansiryah, Baghdad, Iraq.

Using an innovative technique, we created a large area of ultrathin alumina membranes (UTAMs) on silicon substrates to fabricate highly ordered silicon nanoporous arrays and silicon nanowires arrays by wet-chemical etching. Then CdTe is electrochemically deposited on silicon nanowires and silicon nanoporous structures, producing Si-CdTe core-shell nanowires and CdTe-Si core-shell nanostructures, respectively. This approach is aiming at the realization of high efficient solar cells based on Si-CdTe core-shell nanowires. Morphology and crystallization of the resulting core-shell nanowires were investigated by scanning electron microscope, X-ray diffraction and transmission electron microscope. The optical absorption investigation was also carried out for these arrays. The proposed fabrication method is an ef*cient and controllable technique that can be utilized to develop photovoltaic devices of core*shell structures with different compound semiconductor materials.

MM 10: Invited Talk (Hauptvortrag): Schroers

Time: Monday 15:00–15:30 Location: H24

Invited Talk MM 10.1 Mon 15:00 H24

Materials Science and Development of Complex Materials — •Jan Schroers — Yale University, Department of Mechanical Engineering and Materials Science, New Haven, USA

The increasing demands on materials across fields pose a grand challenge. To meet these demands, increasingly complex materials must be developed which requires strategies and techniques to characterize complex materials. We have developed two strategies to address the structural as well as chemical aspects of this challenge. To understand the relationship between materials' properties and chemistry, we have developed effective combinatorial strategies where we employ combinatorial sputtering which allows us to create approximately 800 different alloys simultaneously. High throughput characterization methods have been developed in our lab and are used to determine properties like glass forming ability in metallic glasses, biocompatibility, and electrochemical. Correlating structure with properties is the holy grail of materials science, yet in most cases very difficult to determine accurately. We have developed a technique that allows one to precisely design or replicate and subsequently realize microstructures in materials including metals, polymers, and ceramics, and to manipulate all features individually and independently. Novel materials often require novel processing methods. As an example, we have uncovered novel processing opportunities using thermoplastic forming, which utilize the dramatic yet continuous softening exhibited by a bulk metallic glass as it approaches its glass transition temperature.

MM 11: Topical Session: TEM-Symposium - STEM

Time: Monday 15:45–18:15 Location: H4

Topical Talk MM 11.1 Mon 15:45 H4

Scanning transmission electron microscopy at atomic resolution — •Ferdinand Hofer, Gerald Kothleitner, and Werner Grogger — Institut für Elektronenmikroskopie und Feinstrukturforschung, Technische Universität Graz, Steyrergasse 17, A-8010 Graz, Österreich

Advanced electron microscopy is making a vital contribution to the discoveries taking place in many areas of materials science. Especially, the advantages in aberration corrected TEM and STEM instrumentation now provide necessary background for solving materials science problems at the nanometer or even atomic scale. This is especially true of aberration corrected STEM which brings with it analytical techniques such as electron energy-loss spectroscopy (EELS) and the new silicon drift detector systems for x-ray spectrometry. In this paper we present how modern aberration corrected STEM systems can be used to examine the local chemistry and also the physical properties of energy-related materials, e.g. nanocomposite solar cells, solid oxide fuel cell cathodes and the optical properties of nanoparticles.

MM 11.2 Mon 16:15 H4

High Precision STEM Imaging by Non-Rigid Alignment and Averaging of a Series of Short Exposures — •Paul Voyles[1,2,3], Andrew Yankovich[1], Benjamin Berkels[4], Peter Binev[4], and Wolfgang Dahmen[3] — [1]University of Wisconsin, Madison, United States — [2]Forschungszentrum Jülich, Jülich — [3]RWTH Aachen, Aachen — [4]University of South Carolina, Columbia, South Carolina, United States

We have developed a method for non-rigid registration of a series of Z-contrast scanning transmission electron microscopy (STEM) images. The registered series can be averaged to improve signal to noise without loss of resolution. At very high dose to the sample, 10^5 C/cm^2, lattice images with reproducible precision in the atomic column positions better than 1 pm can be obtained. At an order of magnitude lower dose, images with 2-3 pm precision can be obtained. Lower dose images have been used to measure the displacements of atoms at the edges and corners of Pt on γ-Al_2O_3 nanocatalysts. Edge atoms experience displacements of 10-20 pm, consistent with previous reports. Corner atom displacements are 30-50 pm.

MM 11.3 Mon 16:30 H4

Characterisation of ultrathin ferroelectric film using scannning transmission electron microscopy — •Daesung Park[1], Anja Herpers[2], Tobias Menke[2], Regina Dittmann[2], and Joachim Mayer[1] — [1]Central Facility for electron microscopy (GFE), RWTH Aachen, Germany — [2]Institute of Solid State Research and JARA-FIT, Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Research Center Jülich, Germany

Ferroelectric thin films are attractive candidates for capacitors in random access memory (FeRAM), in which a reversible spontaneous polarisation is utilised to store information. However, below a critical thickness, the ferroelectric property usually disappears. Using smaller in-plane lattice parameter of the substrate induces epitaxial strain which tends to enhance ferroelectric distortion. In this study, niobium doped SrTiO3 is used as a substrate due to its 2.2 % smaller lattice parameter in comparison to BaTiO3. To change and balance the possible mixed termination of BaTiO3, 1.5 additional unit cells of BaRuO3 are embedded between a BaTiO3 thin film (7 unit cells) and SrRuO3 top electrode. The critical thickness depends on the termination of the ferroelectric thin film between electrodes. To elucidate the termination at the interface, high angle annular dark filed (HAADF) imaging and StripeSTEM techniques are carried out in STEM mode due to the high sensitivity to the atomic number Z. Fine structure analysis of Ti-L23 edge is performed to account for Crystal field splitting effect which is a result of the distortion of Perovskite structure.

MM 11.4 Mon 16:45 H4

A transmission electron microscopy study on highly strained BiFeO3 thin films — •Young Heon Kim[1,2], Akash Bhatnagar[1], Ji Hye Lee[1], Marin Alexe[1], Eckhard Pippel[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle (Saale), Germany — [2]Korea Research Institute of Standards and Science, Daejeon 305-340, Republic of Korea

BiFeO3 (BFO) has been widely studied for its astounding magnetoelectric properties, such as antiferromagnetism coupled with ferroelectricity. Although BFO is a rhombohedrally distorted multiferroic perovskite (R3c) in the bulk form, its structural stability is unclear in the form of thin films under strain. The misfit strain by lattice mismatch, one of constraints in thin film growth, causes the distortion of the bulk structure and/or the stabilization of novel phases. Several research groups have recently reported the formation of tetragonally distorted BFO phase (P4mm) on highly-lattice-mismatched substrates. In this talk, we present detailed investigation on the atomic structure and the phase behavior of highly strained BFO thin films, based on a transmission electron microscopy study. The transition information of the rhombohedral to tetragonal-like phase is considered to be a critical issue in achieving highly polarized BFO phase. The morphological and microstructural properties of BFO thin films were studied by various transmission and scanning transmission electron microscopy techniques (specially, with a probe Cs-corrector for atomic resolution in the latter case). We will also show geometrical phase analysis results adopted to determine strain distribution.

MM 11.5 Mon 17:00 H4

Microscopic origin of the giant ferroelectric polarization in strained BiFeO3 thin films — •Marta D. Rossell — Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Because of their astounding electromechanical properties, BiFeO3 (BFO) thin films are promising candidates for the replacement of lead-based ceramics in microelectromechanical system devices. However, a full understanding of the piezoelectric properties reported for these ceramic materials is still missing. In particular, polymorphs of BFO stabilized under epitaxial strain are not yet fully understood. Two distinct structures are known to evolve above and below a 4.5% critical compressive strain. They are pseudotetragonal (T phase) and pseudorhombohedral (R phase), respectively. The T phase shows a unique structure characterized by a strongly elongated unit cell with a c/a axial ratio close to 1.3. The structural information of this metastable polymorph is particularly relevant because it is predicted to have a giant polarization roughly 1.5 times of the bulk material.

We determine the atomic structure of the T phase and the R phase in highly strained BFO thin films by using a combination of atomic-resolution scanning transmission electron microscopy and electron energy-loss spectroscopy (EELS). The coordination of the Fe atoms and their displacement relative to the O and Bi positions are assessed by direct imaging. These observations allow us to interpret the electronic structure data derived from EELS and provide evidence for the giant spontaneous polarization in strained BFO thin films.

MM 11.6 Mon 17:15 H4

STEM HAADF characterization of dilute Bi containing GaAs — •Nikolai Knaub, Andreas Beyer, Peter Ludewig, and Kerstin Volz — Structure and Technology Research Laboratory, Materials Science Center and Faculty of Physics Philipps-Universität Marburg, Germany

Incorporating small amounts of Bi in III/V semiconductors has a huge influence on the energetic position of the valence bands, mainly also of the spin-orbit split-off band. Therefore, dilute bismides such as Ga(AsBi) are promising materials for optical and electronical devices. For a sufficent incorporation of Bi in GaAs, the growth temperature of MOVPE (metal organic vapour phase epitaxy)-grown samples has to be low, typically between 375° C and 450° C. Because of such relatively low growth temperatures point defects, such as Bi or As antisites, can arise and influence the crystal structure. We present the results of STEM (scanning transmission electron microscopy) high angle annular dark field (HAADF) measurements on a MOVPE-grown Ga(AsBi) sample. We used a spherical aberration corrected JEOL JEM 2200 FS with an annular dark field detector for the high resolution. For quantitative comparison with the experimental images, an absorptive potential approximation based simulation software was used for simulations of antisite defects in GaAs and Ga(AsBi). The present contribution will show how to gain information of crystal stochiometry and composition out of experimental as well as simulated HAADF images by using the Voronoi map method. It will be shown that it is possible to describe the influence of point defects on an atomic scale quantitativley.

MM 11.7 Mon 17:30 H4

Analytical transmission electron microscopy in the third dimension — •Bert Freitag, Arda Genc, Jonathan Winterstein, Huikai Cheng, Lee Pullan, and Joerg Jinschek — FEI Company, Eindhoven, The Netherlands

As the feature sizes in material science continue to decrease to nanometer regime, the techniques solely based on 2-dimensional (2D) imaging fail to provide a full characterization of the nanoscale materials. We employed a new tomography technique for STEM XEDS which utilizes the combination of a four silicon drift detector (SDD) system and a high brightness electron gun (XFEG) optimized for high X-ray collection efficiency [1]. Three dimensional tomograms are obtained when the sample is tilted and images and EDS maps are acquired from all angles. The EDS signal can be processed like normal z-contrast images since the EDS signal increases monotonously with the concentration of the element like z-contrast signal increases monotonously with the mass thickness. Examples of 3D chemical mapping using XEDS are given on (InGa)N Nanopyramid LEDs, NiAl3 super alloy material for aircraft turbine blades, high-k dielectric transistor and catalytic particles. In summary, this new technique enables a larger field of view and reduces the acquisition time of a complete XEDS mapping tilt series to hours instead of days, which were impractical before. Even the use of conventionally prepared FIB foils for 3D chemical mapping is possible, which overcomes the difficulties related to background changes with thickness increase known in EELS. [1] P. Schlossmacher et al., Microscopy Today 18(4) (2010) 14-20.

MM 11.8 Mon 17:45 H4

High-resolution HAADF-STEM analysis of hetero-interfaces — •Anna Moros, Harald Rösner, and Gerhard Wilde — WWU Münster

Nanoparticles embedded in an inert immiscible matrix offer ideal conditions to study the impact of hetero-interfaces on reversible phase transitions as for instance melting. Al-Pb composites consisting of nanometer-sized Pb inclusions embedded in a polycrystalline Al matrix serve as model systems for such structural studies. The large lattice constant mismatch of 22.2% between Al and Pb leads to strain at the hetero- matrix-particle interfaces, which is accommodated by misfit dislocations. In order to correlate the thermodynamic properties and the atomic structure of the hetero-interface between the Pb particles and the matrix, an addition of Ga (1 and 3 at. %) selectively into the Al matrix was implemented. Since the lattice constant of the Al(Ga) matrix is extended in comparison with the pure Al matrix, the lattice mismatch between the matrix and the embedded Pb nanoparticles should be reduced. To investigate the interface structure and the particle morphology, aberration-corrected high-resolution HAADF-STEM was performed using the ultra stable stage of the TEAM I microscope. These results will be discussed with the focus on the arrangement of misfit dislocations at the particle-matrix interfaces. The authors acknowledge support of the National Center for Electron Microscopy, Lawrence Berkeley Lab, which is supported by the U.S. Department of Energy under Contract # DE-AC02-05CH11231. Funding by DFG is gratefully acknowledged.

MM 11.9 Mon 18:00 H4

Electrostatic Phase Plates for Transmission Electron Microscopy — •Simon Hettler[1], Manuel Dries[1], Nicole Frindt[2], Rasmus R. Schröder[2], and Dagmar Gerthsen[1] — [1]Laboratorium für Elektronenmikroskopie, KIT, Karlsruhe, Germany — [2]BioQuant CellNetworks, Universität Heidelberg, Heidelberg, Germany

Physical phase plates (PP) for transmission electron microscopy (TEM) enhance phase contrast of (weak-)phase objects by inducing an additional relative phase shift between the scattered and unscattered electrons. The phase shift can be varied by the use of electrostatic PPs, which generate a variable electrostatic field at the zero-order beam position in the back focal plane. An important property of the PP is the cut-on frequency which limits the maximum size of the objects to be imaged with phase contrast. The cut-on frequency is determined by the spatial localization of the electrostatic field which can be optimized by adequate PP design. Moreover, obstruction of scattered electrons in the back focal plane by the PP structure as well as contamination

and charging of the device additionally affect PP TEM.

We implemented a PP optimized in size and shape in a Zeiss 912 Omega transmission electron microscope. The obtained images of different samples show contrast enhancement and inversion. Charging and contamination is minimized using an integrated heating device in the vicinity of the PP. The inhomogeneous potential is analyzed and compared to simulations. The effect of inelastic scattering on phase contrast is studied.

MM 12: Computational Materials Modelling - Mechanical Properties

Time: Monday 15:45–18:15 Location: H24

MM 12.1 Mon 15:45 H24

Self-consistent scale-bridging approach to compute the elasticity of multi-phase polycrystals — •Martin Friak[1], Hajjir Titrian[1,2], Ugur Aydin[1], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Universität Duisburg-Essen, Germany

A necessary prerequisite for a successful theory-guided up-scale design of materials with application-driven elastic properties is the availability of reliable homogenization techniques. We report on a new software tool that enables us to probe and analyze scale-bridging structure-property relations in the elasticity of materials. The newly developed application computes integral elastic response of randomly textured polycrystals. The application employs a Python modular library that uses single-crystalline elastic constants as input parameters and calculates macroscopic elastic moduli (bulk, shear, and Young's) and Poisson ratio of both single-phase and multi-phase aggregates. Crystallites forming the aggregate can be of cubic, tetragonal, hexagonal, orthorhombic, or trigonal symmetry. For cubic polycrystals the method matches the Hershey homogenization scheme. In case of multi-phase polycrystalline composites, the shear moduli are computed as a function of volumetric fractions of phases present in aggregates. Elastic moduli calculated using the analytical self-consistent method are computed together with their bounds as determined by Reuss, Voigt and Hashin-Shtrikman homogenization schemes. The software library can be used as a toolkit for both forward and inverse materials-design strategies.

MM 12.2 Mon 16:00 H24

Mechanical properties of fully lamellar TiAl alloys obtained from a DFT study — •Mansour Kanani, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-University Bochum, 44801 Bochum

Mechanical properties of different interfaces and bulk structures in the fully lamellar TiAl two-phase system are investigated by an ab-initio DFT (Density Functional Theory) based study with full relaxation. Interfacial energies as well as planar fault energies for γ/γ, $\alpha 2/\gamma$ interfaces and bulk structures are calculated. The tensile strength and cohesive properties for different variants are obtained from implementation of atomic scale uni-axial mechanical test. The remarkable finding is that all interfaces as well as bulk phases have comparable normal strengths. Furthermore, shear properties of the single crystals as well as interfaces are investigated on the basis of generalized stacking-fault energy surface and then the shear strength is calculated along various directions. The results show that 60-rotated and 120-rotated γ/γ interfaces display an easy shearing configuration; especially the [-1-12]γ direction shows an invariant and low shear strength for all cases. Our results are discussed and interpreted on the basis of the atomistic configurations of the investigated systems.

MM 12.3 Mon 16:15 H24

Interaction of dislocations with carbon interstitials in α-iron — •Gholamali Nematollahi, Blazej Grabowski, Johann von Pezold, Chris Race, Jörg Neugebauer, and Dierk Raabe — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

The interaction of carbon with dislocations gives rise to the formation of Cottrell atmospheres in α-Fe. This does not only directly affect the mechanical properties of the matrix, but may also result in an indirect effect due to a dislocation-driven rearrangement of the C distribution during severe plastic deformation. Recent experimental studies of severely deformed pearlitic wires reveal a considerable refinement of the cementite layers and a substantial accumulation of C in the ferrite. It was tentatively suggested that the accumulation of C in the ferritic layers proceeds via the co-migration of C atoms with mobile dislocations gliding from the ferrite/cementite interface into the ferrite phase. In the present study, we provide molecular statics calculations addressing the proposed mechanism in detail. In particular, nudged elastic band (NEB) calculations are used to determine the effective migration barrier for an interstitial C atom in the vicinity of an edge and screw dislocation in α-Fe, using a semi-empirical EAM potential. Carbon diffusion barriers of 0.2 eV are found in the core of the dislocation suggesting that carbon is more mobile than in bulk iron (barrier: 0.9 eV). The Portevin-le Chatelier effect that suggests the mobile solute atoms can diffuse with the moving dislocation at high temperature and moderate strain rate. These conditions are satisfied about C in the dislocation core already at room temperature.

MM 12.4 Mon 16:30 H24

Atomistic modelling of α-Fe and Fe-C by analytic bond-order potentials including magnetism — •Sebastian Schreiber, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum

The mechanical properties of steels are to a large degree determined by plastic deformations on the microstructural level. Understanding the involved processes at such length-scales calls for atomistic simulations of the movement of line defects. This may help to explain, e.g., the influence of temperature and carbon content on dislocation glide in α-Fe and to make direct contact to recent atom-probe experiments. However, simulating the interaction of dislocations and other defects with atomic resolution requires computationally efficient methods that are able to treat million-atom simulation cells. To this end, we develop analytic Bond-Order potentials (BOP) that are footed on recently parametrised tight-binding (TB) models of Fe and Fe-C. The analytic BOP provide an approximate solution to the TB problem and include the treatment of magnetism within the Stoner model. Here, we demonstrate the transferability of taking the Fe and Fe-C TB parameters to the analytic BOP formalism and discuss first results of large scale BOP simulations that will lead us to the calculation of the Peierls stress for dislocation movement. Moreover, we will present benchmarks of the computational performance of the analytic BOP with respect to system size and parallelisation.

MM 12.5 Mon 16:45 H24

First-principles calculations of the key atomistic parameters related to hydrogen embrittlement in FeMn — •Aurab Chakrabarty, Johann von Pezold, Robert Spatschek, Tilmann Hickel, and Joerg Neugebauer — Max-Planck Institute for Iron Research, Duesseldorf, Germany

Hydrogen embrittlement in high-manganese steels has been in the centre of attention for automotive applications. It is difficult to perceive the role of hydrogen of these steels solely from experiments. However, key atomistic parameters such as H-H interaction, elastic constants, solution energies and stacking fault energies can be systematically determined from first-principles calculations. They can be used to create a fully ab-initio based continuum scale simulation and validate commonly assumed assumptions of H-segregation on stacking faults, cracktips and cleavages and eventually to understand phenomena such as HELP (hydrogen enhanced local plasticity).

In this work we apply density functional theory to investigate the role of hydrogen in FeMn. Starting with the crystal and magnetic structure for H-interstitials, we calculated the hydrogen solution energy in a hydride phase and H-H interactions in Fe and Mn in order to investigate the possibility of hydrogen congregation. The energetic preferences of the interstitial sites for a hydrogen atom in Fe-Mn alloy based on the number of Fe/Mn neighbours, have been determined. These parameters, including their chemical and elastic contributions were analyzed in order to understand the nature of the defect and implications for alloys those are less sensitive to H-embrittlement.

MM 12.6 Mon 17:00 H24

Shear instabilities in perfect bcc crystals during simulated tensile tests — •Miroslav Černý[1,2], Petr Šesták[1,2], Jaroslav

Pokluda[2], and Mojmír Šob[1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Faculty of Science, Masaryk University, Brno, Czech Republic

This work demonstrates a simple but efficient way how to determine the existence of shear instabilities in ideal bcc crystals under uniaxial loading. The theoretical tensile strengths are derived from calculated values of the theoretical shear strength and their dependence on the superimposed normal stress. The presented procedure enables us to avoid complicated and time-consuming analyses of elastic stability of crystals. Results of first-principles simulations of coupled shear and tensile deformations for two most frequent slip systems ($\{110\}\langle 111\rangle$ and $\{112\}\langle 111\rangle$) in six ideal cubic crystals are used to evaluate the uniaxial tensile strengths in three low-index crystallographic directions ($\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$) by assuming a shear instability in the weakest shear system. While instabilities occurring under $\langle 100\rangle$ tension are mostly related to the shear in $\{112\}$ plane, those occurring during loading in the other two directions are associated with $\{110\}$ planes. The results are consistent with those predicted by available elastic analyses. The weakest tendency to fail by shear is predicted for uniaxial tension along $\langle 100\rangle$. This is consistent with occurrence of $\{100\}$ cleavage planes in bcc metals.

MM 12.7 Mon 17:15 H24

Modeling of pressure-induced phase transformation in Si using a two phases strategy — Sebastien Groh, •Michael Budnitsky, and Meinhard Kuna — TU Bergakademie Freiberg, Freiberg, Germany

We have carried out constant pressure molecular dynamics simulation with a Tersoff interatomic potential to study the pressure-induced phase transformation in Si using a two-phases model. The simulations successfully reproduced the diamond-cubic to β-Sn structural transformation under hydrostatic pressure. The pressure level at which the transformation occurred is in agreement with both experimental data and thermodynamics considerations. Moreover, the mechanism of phase transformation by inhomogeneous shear deformation was revealed by the calculations. Furthermore, as the β-Sn cannot transform back to diamond-cubic structure, it was observed in the simulation that the two-phases model transformed to a diamond- cubic and an amorphous Si for pressure lower than the transition pressure. Although such a transformation from β-Sn to amorphous Si was already observed by simulation of nanoindentation of Si using MD, it is the first that time this transformation is reported under hydrostatic loading conditions using molecular dynamics simulations.

MM 12.8 Mon 17:30 H24

Extended Modules Material Assembly — •Matthew S Dyer, Christopher Collins, Darren Hodgeman, Philip Chater, Antoine Demont, Simon Romani, Ruth Sayers, Michael F Thomas, John B Claridge, George R Darling, and Matthew J Rosseinsky — University of Liverpool, Liverpool, UK

Computational approaches have a growing influence on the search for new materials. However, potential functional materials with complex structures still pose the problem of an excessive number of permutations needing consideration and screening. Here we present the Extended Modules Material Assembly (EMMA) method to address this issue. EMMA constructs a set of structures based on layered building blocks, combined using predefined rules.

In the present study, we investigate layered perovskite oxides within the Y-Ba-Ca-Fe-Cu-O phase diagram. A new material was identified, synthesised, and its structure determined using a combination of the EMMA method and experimental diffraction methods. This complex structure has 6 elements in 20 distinct sites, and a longest lattice constant of 61 Å. We have shown experimentally that the new material is a functional cathode for solid oxide fuel cells.

Many functional materials, even those with complicated structures, can be described as a periodic combination of constituent layers. The EMMA method is particularly well suited to these materials, where brute force approaches cannot be used and chemical knowledge needs to be used to guide structural searches. It is a pragmatic, practical method aiding the discovery of new functional materials.

MM 12.9 Mon 17:45 H24

Massively parallel detection of contacts for packing problems using NVIDIA CUDA — •Jakob Nixdorf and Eckard Specht — Otto-von-Guericke-University Magdeburg, Department of Experimental Physics/Material Physics

High density packings of particles are often used as models of the structure of liquid, glassy and crystalline states of matter, granular media, heterogeneous materials and even biological systems.

In this work the packing of millions of unequal spheres is studied. The crucial and by far most time-consuming part of such computer simulations is the detection of contacts and overlaps between the spheres and the container. A massively parallel approach has been implemented using the CUDA toolkit for programming NVIDIA Tesla graphics cards. Problems and results of this implementation are discussed and compared with a serial implementation as well as the efforts of other groups.

MM 12.10 Mon 18:00 H24

Direction Dependent Field Evaporation of Pure Materials in Atom Probe Tomography — •Torben Boll and Talaat Al-Kassab — King Abdullah University of Science and Technology, Division of Physical Sciences and Engineering, Thuwal, 23955-6900, Saudi Arabia

In the field of atom probe tomography (APT) the process of field evaporation governs the progress of an analysis. The field evaporation field (FEF) is known to exhibit different strengths for different crystallographic directions for pure metals. However this is not considered in currently used APT-models. This paper will present a method to calculate small differences in the FEF for crystallographic directions from experimental APT data of Al, W and Si. Furthermore we will discuss how this can be used to adjust parameters for geometry based APT-simulations.

To obtain this information we developed an upgraded version of the AtomVicinity algorithm, which is mostly identical to what is also called *spatial distribution maps*.

The results were acquired with two different commercial atom probes, the Laser assisted Wide Angle Atom Probe (LA-WATAP) and the Local Electrode Atom Probe (LEAP 4000). Additionally, this approach allows a comparison of the spatial resolution of these two devices.

MM 13: Topical Session: Quasicrystals & Complex Metallic Alloys III

Time: Monday 15:45–18:00 Location: H25

MM 13.1 Mon 15:45 H25

Dealing with the complexity of complex matter — •Peter Häussler — University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Describing the structure of complex systems is difficult enough but, due to the huge unit cell and unknown decoration of the lattice sites, what often happens, calculating their properties is even worse. Understanding their structural evolution from e.g. the gaseous or liquid state and the reasons where structural peaks finally arise is far out of this range. One way, to reduce the tremendous number of parameters and hence to understand their structural development as well as the evolution of physical properties, is to give up a microscopic understanding based on a detailed description of all the individual atoms. We may even ask, is it really necessary to know all these details which we may, probably, never be able to get? Can we tread the complexity with reduced information? If we are able to find global subsystems, consisting of many species which are acting collectively, we would be able to reduce the tremendous number of independent parameters to a few only. If we are further able to describe with these parameters the major effects causing the atomic distances as well as main physical properties, we may have understood a lot. I will talk in this presentation on global effects of different subgroups of electrons. The combined s/p-electrons, the s-electrons alone, as well as the d-electrons, all have their own effects on structural features. Together with the structure they cause the metallic, insulating or semiconducting properties, are

defining the atomic density and many more quantities.

MM 13.2 Mon 16:00 H25

Single-crystal growth of various complex metallic alloy phases — •Michael Feuerbacher, Marc Heggen, and Carsten Thomas — Forschungszentrum Juelich, 52349 Juelich, Germany

Complex metallic alloys (CMAs) are intermetallic compounds with large lattice parameters and unit cells containing some tens to some thousands of atoms. Their local order is in most cases dominated by icosahedral atom coordination, which distinguishes CMAs from simple metals and compounds. In order to be able to establish intrinsic structure-property relations characteristic of the particular local order, the availability of high-quality single crystals is of particular importance. In this presentation we report on single-crystal growth approaches on various different, mostly Al-based CMAs. We present the growth techniques applied and the resulting single crystals along with critical primary characterizations. The strategy of phase selection, which is essential to achieve comprehensive structure-property relations by comparative studies, is discussed.

MM 13.3 Mon 16:15 H25

Metadislocation core structure in the complex metallic alloy $Al_{13}Co_4$ — •Marc Heggen and Michael Feuerbacher — Peter Grünberg Institut, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

We have analysed metadislocations in the complex alloy $Al_{13}Co_4$. The core structure is studied using aberration-corrected high-resolution scanning transmission electron microscopy. Different types of metadislocations with Burgers vectors of b = +/-tau^{-n} b (0 1 0) (n = 3, 4) are found which are associated to four and six planar defects, respectively. They are escorted by phason defects and move, in contrast to metadislocations in most other complex alloys, by pure glide.

MM 13.4 Mon 16:30 H25

Structure of a decagonal Al–Pd–Mn quasicrystal with 16 Å periodicity — •Benjamin Frigan[1], Marek Mihalkovič[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

We present the first detailed structure solution for a decagonal quasicrystal in the Al–Pd–Mn system by means of *ab initio* energy minimization. It is based on structure models of the ε_6- and other approximant phases. All phases consist of columns of pseudo-Mackay icosahedra (PMI), whose projections form tilings of the plane. In between there are glue atoms in the form of large bicapped pentagonal prisms (LBPP). In the past, we have optimized the structure of the ε-phases, where the tilings consist of pentagons, hexagons and nonagons. These can be represented as subsets of a hexagon-boat-star (HBS) tiling. The decagonal phase comprises further HBS-tiles. We have constructed several HBS approximants and decorated them with PMI and LBPP clusters. Whereas the PMI clusters were kept essentially unchanged, each LBPP is adjusted in occupancy depending on its position in the various tiles. In this way we obtain cluster decorations for all tiles of the decagonal quasicrystal. The structures were optimized by molecular dynamics annealing with specially developed EAM-potentials, followed by further relaxation with *ab initio* calculations. The quality of the structures is judged by their position within the convex hull of stable, experimentally known phases of the Al–Pd–Mn phase diagram.

MM 13.5 Mon 16:45 H25

Cu–Sn Cluster Compounds — •Saskia Stegmaier, Thomas F. Fässler, and Karsten Reuter — Technische Universität München, Germany

Nanostructured intermetallic materials attract wide interest because of their structural and physical properties and the related potential for applications, for example in catalysis or electronics.
The intermetallic compounds $A_{12}Cu_{12}Sn_{21}$ (A = Na, K, Rb, Cs) [1] and $Na_{2.8}Cu_5Sn_{5.6}$ [2] feature intriguing new Cu–Sn cluster species. These are onion-skin-like $\{Sn@Cu_{12}@Sn_{20}\}$ clusters with quasi-icosahedral symmetry and related pseudo-five-fold symmetric $^1_\infty\{Sn_{0.6}@Cu_5@Sn_5\}$ rods, respectively. In the solid state structures of the A–Cu–Sn phases the polyanionic Cu–Sn clusters or rods are separated from each other by alkali metal cations. The ternary phases thus represent promising precursors for the synthesis of new nanostructured binary Cu–Sn materials.
In view of this perspective we perform density functional theory calculations to computationally search for such potential Cu–Sn compounds—including discrete clusters and wires, as well as 3D periodic structures.

[1] S. Stegmaier, T. F. Fässler, *J. Am. Chem. Soc.* **2011**, *133*, 19758.
[2] S. Stegmaier, T. F. Fässler, *Angew. Chem. Int. Ed.* **2012**, *51*, 2647.

MM 13.6 Mon 17:00 H25

Thermal Conductivity in Type-I Clathrate Systems — •Daniel Schopf and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart

Intermetallic clathrates are currently actively investigated due to their special thermoelectric properties. They are composed of periodically arranged cages, formed by host atoms, which enclose single guest atoms. The low thermal conductivity of these structures has been attributed to the scattering of the phonons on the local vibration modes ("rattling") of these guest atoms.

Molecular dynamics simulations can be used to study the influence of complexity on the thermal conductivity. To model the strongly directional atomic interactions in clathrates, angular dependent potentials are required. Effective potentials have been determined with the force-matching method and will be presented.

The Green-Kubo method has been used to calculate the thermal conductivity of clathrate systems with different levels of complexity. The influence of the size of the unit cell and the arrangement of vacancies as sources of the low conductivity are discussed.

MM 13.7 Mon 17:15 H25

Medium-range structure of $Zr_{50}Cu_{45}Al_5$ Bulk Metallic Glass from Fluctuation Electron Microscopy — •Paul Voyles[1,2,3], Jinwoo Hwang[1], Zenon Melgarejo[1], Irena Kalay[4], Eren Kalay[4], Matt Kramer[4], and Don Stone[1] — [1]University of Wisconsin, Madison, United States — [2]Forschungszentrum Jülich, Jülich — [3]RWTH Aachen, Aachen — [4]Ames Lab, Iowa, United States

By combining fluctuation electron microscopy data sensitive to medium-range order (MRO) with an empirical interatomic potential sensitive to short-range order (SRO) in a single hybrid reverse Monte Carlo structural refinement, we have found two types of structural order in $Zr_{50}Cu_{45}Al_5$ bulk metallic glass [1]. One structure consists of icosahedral nearest-neighbor SRO clusters, arranged in chains at the MRO length scale of 1 nm. The other structure is more crystal-like, consisting of SRO clusters with more 4- and 6-sided faces on their Voronoi polyhedra. The crystal-like SRO clusters organize into compact MRO clusters with distinct 4- and 6-fold rotational symmetry. Experimentally, structural relaxation shifts the cluster population from crystal-like to more icosahedral. In molecular dynamics, the structural models are stable under annealing at temperatures well below T_g. The structural evolution of the models through the simulated glass transition will be discussed.

[1] J. Hwang, Z. Melgarejo, Y. Kalay, I. Kalay, M. J. Kramer, D. S. Stone, P. M. Voyles, Phys. Rev. Lett. 108, 195505 (2012)

MM 13.8 Mon 17:30 H25

How atomic structure forms - a general principle — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

The evolution of atomic structure on large scales is still not well understood. In principle one has to deal with approximately 10^{23} individual atoms, but even a few hundreds are still too much to apply microscopic techniques - the number of parameters would still be horrible. Subsequently, one is left with simulations and techniques which implement the final results in advance. On the other hand, we observed that structure formation is to a great extent an ordering process where a few global subsystems, like the outer electrons as one, and the remaining ions as the other one, are behaving collectively. Both are connected by global resonances. Using collectivity allows the reduction of the number of independent parameters to a few only - to understand the most important principle, the formation of gaps or pseudo gaps at the Fermi energy. Redistributing electrons at the Fermi energy causes very effective reductions of the total energy of the system and, hence, stabilizes particular structures. I will talk about this principle for completely different systems as all the liquid elements along the periodic table (molecular and elemental liquids, liquid insulators, metals, or semiconductors), and the rising complexity, whenever alloys have to

be understood. Complexities as charge transfer, hybridization effects, phase separation, the formation of quasi- or nano-crystalline inclusions are described as well. We became able to predict mayor structural motif of not yet measured systems and their electronic properties

MM 13.9 Mon 17:45 H25

On the evolution of structure and electronic transport properties in Al-Mn — •Syed Sajid Ali Gillani and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

A systematic study of thin films of Al-Mn, evaporated at T=4 K, shows mixtures of amorphous, quasi-crystalline, as well as nano-crystalline phases. Their structures have been investigated by electron diffraction, their transport properties and thermal stability by resistivity measurements, indicating clear evidences of resonance effects between global subsystems as there are the Fermi gas as one, and the forming static structure as the other one. The global resonances are self-organizing via their exchange of characteristic momenta and angular momenta, respectively and dominate all the properties including phase stability and phase separation. The amorphous phase shows in r-space spherical periodic order, predominately based on an exchange of characteristic momenta alone. Al-rich alloys show, in addition, features of quasi-crystalline order and Mn-rich alloys an enhanced content of nano-crystalline periodic order. The characteristic distances between theses phases are related among each other and to half the Fermi wavelength λ_F, indicating resonance effects in all of them. In k-space the corresponding structure factor $S(K)$ shows a resonance peak at scattering vector $K_{pe} = 2k_F$ with an additional prepeak in the range of the quasi-crystalline phase and further peaks in the range of enhanced nano-crystallinity.

MM 14: Functional Materials - Hydrogen

Time: Monday 15:45–18:15 Location: H26

MM 14.1 Mon 15:45 H26

Design and synthesis of core/shell SnO_2/MnO_2 nanotube arrays for high performance supercapacitor application — •Fabian Grote, Huaping Zhao, Ranjith Vellacheri, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany.

Recently, we focused on the development of nanostructured three-dimensional electrode materials for applications in supercapacitor devices. Therefore, we developed a synthesis process to fabricate nanostructured free-standing core/shell SnO_2/MnO_2 nanotube arrays. The core/shell nanotube arrays were prepared by atomic layer deposition (ALD) of SnO_2 into porous alumina membranes and a subsequent coating by MnO_2. The essential features of this structure are its high surface area, hollow nature of the structure, good conformal coating of the SnO_2 nanotubes with MnO_2, and the desired core/shell structure. The electrochemical performance of the prepared electrodes was studied in CV, charge/discharge, and long-term cycle stability experiments and exhibited excellent performance. These results so far address key challenges of supercapacitors and shall pave the way to realize a high performance supercapacitor with not only high power density, but also high energy density. For further investigation the morphology of the core/shell SnO_2/MnO_2 nanotube arrays was analyzed by SEM and TEM. The chemical composition was determined by XPS, EELS, and XRD measurements.

MM 14.2 Mon 16:00 H26

High-performance supercapacitors based on orderd nanoarrays — •Ranjith Vellacheri, Huaping Zhao, Ahmed Al-Haddad, Fabian Grote, and Yong Lei — Fachgebiet 3D-Nanostrukturierung , Institute fur Physik & IMN MacroNano (ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

Supercapacitors are electrochemical energy storage devices potentially useful for high power demanding applications. Three-dimensional nanostructures of metal oxides and conducting polymers are considered as promising candidates for the development of high-performance supercpacitor electrodes. Here, we will discuss about the preparation of different kinds of nanoarrays such as nanotube arrays and core-shell nanowire arrays, by using anodic alumina nano-templates. Alumina templates can be employed to make well ordered three-dimensional nanostructures with superior surface properties. Our strategies mainly include the preparation of MnO2 and PEDOT nanotube arrays, Ni-NiCo2O4 core-shell nanowire arrays and NiCo2O4-TiO2-NiCo2O4 sandwich-structured nanotube arrays, and the fabrication of supercapacitors by utilizing these nanoarrays shall be useful for wide range of applications.

MM 14.3 Mon 16:15 H26

Nano-engineered three-dimensional Pt/MnO2 thin films for flexible, high performance supercapacitors — •liaoyong wen, yan mi, fabian grote, ahmed al haddad, zhibing zhan, huaping zhao, and yong lei — Institut für Physik & IMN MacroNano* (ZIK), Institute for Physics and IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Supercapacitors, also called ultracapacitors or electrochemical capacitors (ECs), have become some of the most promising candidates for next-generation power devices because of their high power density, fast charging-discharging rate, and excellent cycle stability. Manganese Oxide (MnO2), owing to its high theoretical specific capacitance, has been considered to be one of the most attractive electrode materials for supercapacitors. Here we construct mechanically flexible three-dimensional thin film supercapacitors by assembling nano-engineered Pt/MnO2 electrodes, prepared in anodic alumina nano-porous templates with Atomic Layer Deposition (ALD) technology and electrodeposition process. The well-defined three-dimensional Pt nanostructures, acting as electrodes and also current collectors, address the inherit disadvantage of the poor electrical conductivity (10-5*10-6 S/cm) of MnO2. Meanwhile, the nanostructured morphology of the Pt electrode can provide very large surface, which largely enhance the energy and power density of the supercapacitors. The much improved performance (energy and power density) and excellent mechanical flexibility of the supecapacitor make it a unique design in various power delivery applications.

MM 14.4 Mon 16:30 H26

Synthesis and characterization of nanoparticulate $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ cathodes for thin film solid oxide fuel cells — •Cahit Benel[1,2,3], Azad J. Darbandi[1,2], Anna Evans[4], René Tölke[4], Michel Prestat[4], and Horst Hahn[1,2] — [1]Institute for Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt and Karlsruhe Institute of Technology, Germany — [3]Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [4]Nonmetallic Inorganic Materials, ETH Zurich, Switzerland

Solid oxide fuel cell cathode materials with mixed ionic and electronic conductivity (MIEC) such as strontium doped lanthanum cobalt oxide ($La_{0.6}Sr_{0.4}CoO_{3-\delta}$) show enhanced oxygen reduction kinetics compared to the conventional cathode materials. In this work, nanocrystalline $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ (LSC) powder with ultrafine microstructure and high specific surface area (60 m^2/g) was synthesized via salt-assisted spray pyrolysis method. Nanoparticulate cathode thin films of LSC and LSC-GDC (Gadolinium doped ceria) with thicknesses between 150 and 500 nm were prepared via single step spin coating of water-based nanodispersions on yttria stabilized zirconia (YSZ) substrates. LSC cathode thin films (250 nm) with 30 wt% GDC content exhibit the lowest area specific resistance (ASR) values of 0.32, 0.78 and 2.04 $\Omega.cm^2$ in ambient air at 650, 600 and 550 °C, respectively. The future work will focus on detailed chemical and microstructural analysis of the nanoparticulate thin film cathodes to gain more understanding on the electrochemical processes.

MM 14.5 Mon 16:45 H26

Diffusion of hydrogen in strained Fe and Ni lattices — •Davide Di Stefano, Matous Mrovec, and Christian Elsaesser — Fraunhofer Institute For Mechanics Of Materials IWM, Freiburg, Germany

A correct description for the diffusion of hydrogen in metals is prerequisite for understanding the phenomenon of hydrogen embrittle-

ment. The H diffusion in bulk materials has been studied extensively in the past both experimentally and theoretically. Nevertheless, the knowledge of diffusion processes in distorted environments, e.g. in the vicinity of crystal defects, is still limited.

In this comparative study, we perform atomistic calculations of diffusion barriers in strained structures of Fe and Ni using accurate first-principles methods based on the density functional theory and semi-empirical tight binding. Our results show that the diffusion barriers are indeed strongly influenced by the lattice distortions and depend sensitively on the type of deformation. In addition, our analysis confirms that a proper treatment of quantum effects is crucial for a reliable theoretical determination of the diffusion barriers.

MM 14.6 Mon 17:00 H26

Influence of hydrogen on Gd(0001) thin films — •Sara Wanjelik, Volkmar Hess, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Hydrogen in metals as an area of research has been of great interest for the past few decades. But only few investigations are carried out by imaging techniques with resolution on the nm-scale. Even less works deal with the inital stage of hydride formation.

Here we present STM measurements on thin Gadolinium films grown on a W(110) surface concentrating on the inital steps of hydrogen absorption. Due to the existence of a surface state only on the clean Gd(0001) surface, hydrogen covered areas appear lower in the topography image. Consequently, we can estimate the coverage and the time being necessary for absorption due to the reappearance of the surface state. Our measurements show that there is a lower limit for the amount of hydrogen to initiate the absorption process.

With increasing absorption hydride formation occurs. The larger volume of the hydride results in plastic deformations. On the one hand, there are disk-like islands with a diameter of approximately 3 nm and a height of 0.3 nm, while on the other hand there are coherent areas formed by ramps. The islands were found to arrange in chains. Therefore, we concentrate particularly on the direction of the chains being indicative for crystallographic properties inside the film.

MM 14.7 Mon 17:15 H26

In-situ EELS studies on the dehydrogenation of nanocrystalline MgH_2 — •Alexander Surrey[1,2], Inge Lindemann[1,2], Christian Bonatto Minella[1], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institut fur Festkörperphysik, D-01062 Dresden, Germany

In the field of hydrogen storage there is a still ongoing search for a material that provides both high H_2 storage density and good H_2 sorption properties. Here, nanosized or nanoconfined hydrides promise improved thermodynamics and kinetics. As for the structural characterization utilizing TEM, however, most materials degrade fast upon the irradiation with the imaging electron beam due to radiolysis. MgH_2 is one of the best studied binary hydrides due to its relatively high storage capacity of 7.6 wt.% H_2. Therefore, ball milled MgH_2 was used as a reference material for in-situ TEM experiments on submicron particles. Hereto, EELS measurements were conducted in an aberration-corrected FEI Titan^3 80-300 microscope. From an observation of the plasmonic absorptions it is found that MgH_2 successively converts into Mg upon electron irradiation. The temporal evolution of the spectra is analyzed quantitatively to determine the fractions of pure and hydrogenated Mg at different stages of the reaction and to determine the critical electron doses for both incident electron energies of 80 keV and 300 keV. By comparing these critical doses the dehydrogenation kinetics of individual particles can be investigated. This understanding is also crucial for TEM studies on other hydrides such as AlH_3.

MM 14.8 Mon 17:30 H26

Hydrogen Retention in Metals — •Katrin Peeper[1], Marcus Moser[1], Patrick Reichart[1], Elena Markina[2], Matej Mayer[2], Zhijie Jiao[3], and Gary Was[3] — [1]Universität der Bundeswehr, Angewandte Physik und Messtechnik, München, Germany — [2]Max-Planck-Institute for Plasma Physics, EURATOM Association, Garching, Germany — [3]Department of Engineering and Radiological Sciences, College of Engineering, University of Michigan, Ann Arbor, MI, USA

Degradation of wall materials used in fission and fusion reactors due to extreme conditions and radiation is investigated in order to develop improved materials. Hydrogen plays a key role in metal embrittlement and is trapped at various natural and ion induced defects. We present detailed study of the hydrogen retention in tungsten in 3 dimensions and its correlation with structural features e.g. grain boundaries and blisters performed by proton-proton-scattering.

We show that we obtain a sensitivity better than 10^15 at/cm^2 (2 at-ppm) in metals. We utilised 22 MeV protons to study hydrogen distributions in 50 um Stainless Steel and 25 um Tungsten samples. The steel samples have been irradiated with 2 MeV protons. The depth profiles show that less than 0.3% of the implanted hydrogen is retained and is localized mostly in the end of range peak. The Tungsten samples have been implanted using a Hydrogen ion beam with the energy of 200 eV/H. At these conditions, which mimic the conditions in future fusion reactors, blisters and cracks are created in the near-surface layer due to hydrogen-induced stress in the material.

MM 14.9 Mon 17:45 H26

Quantitative 3D Microscopy of Hydrogen by Proton-Proton Scattering — •Marcus Moser[1], Stefan Wagner[2], Katrin Peeper[1], Patrick Reichart[1], Astrid Pundt[2] und Günther Dollinger[1] — [1]Universität der Bundeswehr München, 85579 Neubiberg, Germany — [2]Institut für Materialphysik, Universität Göttingen, Göttingen 37077, Germany

Proton-proton scattering at the Munich microprobe SNAKE gives the unique possibility for sensitive 3D hydrogen microscopy [1]. Quantification of the hydrogen content without the need of any reference sample, a sensitivity of few or even less than one atomic part per million, a lateral resolution of about 1 *m and a depth resolution of a few micrometers are the main characteristics. We use proton energies between 10 MeV and 25 MeV for analyzing any kind of unsupported samples with thickness between 10 um and 250 um depending on the atomic density of the investigated material. With this method, we measured hydrogen in thin Nb-films. The Nb- films with a thickness of 700nm are electrochemically doped with hydrogen. We have been able to detect and quantify lateral hydrogen distributions and variations induced by hydrogen charging. Hydrogen within the crystallites was measured to be below 0.08 at-ppm.

References [1] P. Reichart, et al., Science 306 (2004) 1537.

MM 14.10 Mon 18:00 H26

Changes in the Electronic Structure of Deuterium Implanted Molybdenum and Rhodium — •Baran Eren, Laurent Marot, Marco Wisse, Roland Steiner, and Ernst Meyer — Klingelbergstrasse 82 4056 Basel Schweiz

In this presentation, two recent works of our group are going to be presented. In the first work molybdenum coatings and in the second work rhodium coatings were treated with low temperature deuterium plasma. Both are considered as candidates as light reflection components in the next generation fusion reactors, therefore changes in their electronic properties may be important for the optical diagnostic systems.

It is shown that hydrogen acts as an electron acceptor in molybdenum, but an electron donor in rhodium. Both cases are investigated with various experimental techniques including photoelectron spectroscopy, spectroscopic ellipsometry, spectroscopic reflectometry, spectrophotometry, specific resisvity and direct surface morphology imaging techniques. Rhodium/hydrogen system is not stable in air due to a catalytic reaction between hydrogen and oxygen, whereas molybdenum/hydrogen system is stable because hydrogen is strongly bound to defect sites.

MM 15: Poster Session

Time: Monday 18:00–20:00 Location: Poster E

MM 15.1 Mon 18:00 Poster E

Precipitate Formation in Fe-Cu Systems investigated by Computer Simulations — •Johannes Zeman[1], Kai Kratzer[1], David Molnar[2], and Axel Arnold[1] — [1]ICP, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]IMWF, Universität Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany

At temperatures above 300°C, copper-alloyed bcc-iron relatively quickly shows the formation of copper nanoprecipitates strongly affecting its mechanical properties. We investigate the kinetics of this phase transition qualitatively and quantitatively, using a vacancy-based atomistic kinetic Monte-Carlo simulation [1]. At high supersaturations, we find that Ostwald ripening is the dominant process, while at low supersaturations, nucleation determines the overall time scale of the transition. The time-temperature- transformation analysis [2] on the whole range of temperatures therefore requires the combination of brute force simulations and forward flux rare event sampling [3]. Our simulations show good agreement with the Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory.

[1] P. Binkele: Atomistische Modellierung und Computersimulation der Ostwald-Reifung von Ausscheidungen beim Einsatz von kupferhaltigen Stählen, PhD thesis, University of Stuttgart (2006)

[2] E. J. Mittemeijer: Fundamentals of Materials Science, p. 426, Springer, Heidelberg (2011)

[3] R. J. Allen, C. Valeriani, and P. Rein ten Wolde: Forward flux sampling for rare event simulations, J. Phys. Condens. Matter 21 (2009)

MM 15.2 Mon 18:00 Poster E

Grain boundary chemistry in nickel alloys applied in 700°C coal-power plant — •Miriam Magdalena Lange[1], Sergiy Borodin[1], Michael Spiegel[2], and Frank Uwe Renner[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Department for Interface Chemistry and Surface Engineering, Düsseldorf, Germany — [2]Salzgitter Mannesmann Forschung GmbH, Duisburg, Germany

Nickel-based alloys are highly interesting materials for application in the new technology of 700°C coal-power plants. Compared to conventional power plants the temperature is increased from 600°C to 700°C at a pressure of 350 bar. During first tests under flue gas atmosphere and pressurized steam the nickel-based alloys showed significant grain boundary sulfidation. The grain boundary chemistry before and after sulfidation under high-temperature working conditions of specific variants of Alloy 617 and corresponding model casts have been investigated by means of Auger Electron Spectroscopy (AES), accompanied by conventional surface analysis. Understanding the mechanisms of grain boundary sulfidation as a result of a specific grain boundary chemistry of these materials can help to improve their corrosion resistance by grain boundary engineering. Initial results on the investigation of grain boundary chemistry of Alloy 617 before and after sulfidation will be presented.

MM 15.3 Mon 18:00 Poster E

Projection potentials and total energy convergence in the KKR method — •Rudolf Zeller — IAS-3, Forschungszentrum Juelich

Although the full-potential Korringa-Kohn-Rostoker Green function method yields accurate results for many physical properties, the convergence of calculated total energies with respect to the angular momentum cutoff is usually considered to be less satisfactory. This is surprising because accurate single-particle energies are expected if they are calculated by Lloyd's formula and because accurate densities and hence accurate double-counting energies should result from the total energy variational principle. It is shown how the concept of projection potentials can be used as a tool to analyse the convergence behaviour. The key factor blocking fast convergence is identified and it is illustrated how total energies can be improved with only a modest increase of computing time.

MM 15.4 Mon 18:00 Poster E

Mechanical and magnetic properties of Fe-Cu and Ni-Cu nanocomposites — •Tomáš Káňa[1] and Mojmír Šob[2,1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Using ab initio calculations, we predict theoretical tensile strength of Fe-Cu and Ni-Cu nanocomposites consisting of Fe or Ni nanowires embedded in the Cu matrix along the [100] direction; simulation of tensile and compressive tests is performed along this direction. We find that the presence of Fe nanowires enhances the maximum deformation in tension and diminish the maximum stress in compression. On the other hand, Fe nanowires do not affect the maximum stress in tension. The preferred mutual magnetic ordering of the nanowires is antiferromagnetic (AFM) one with parallel orientation of all spins in each individual nanowire. The energy gain of this AFM ordering decreases with increasing distance of Fe nanowires. Ni nanowires in Cu matrix do not affect the maximum deformation but enhance the maximum stress in tension. No magnetic ordering of Ni nanowires was found.

MM 15.5 Mon 18:00 Poster E

Cation -Anion interactions, Noncentrosymmetry vs Centrosymmetry : A first-principles study — •Abhishek Kumar Mishra[1], Kenneth V. Poeppelmeier[2], and Umesh V. Waghmare[1] — [1]Theoretical Sciences Unit, J Nehru Centre for Advanced Scientific Research, Bangalore-560064, INDIA — [2]Departments of Chemistry, Northwestern University, Evanston, Illinois, 60208-3113

Materials with non-centrosymmetric (NC) structure posses different technologically important physical properties such as piezoelectricity, ferroelectricty and pyroelectricity due to their symmetry dependent properties. These properties make them find applications in different fields viz. burglar alarms, pollution monitors, thermal detectors, multifunctional devices, photonics technology. Several interesting interrelationships occur between the symmetry-dependent properties and that is why these materials are of special interest in materials chemistry.

We present a theoretical study of structure-property correlation in noncentrosymmetric KNaNbOF5 and centrosymmetric CsNaNbOF5, based on first principles calculations followed by subsequent comparison with experiments. We have worked on stability, electronic and polar properties of these structures and on their solid solutions. Electronic density of states calculations reveals specific bands responsible for breaking of centrosymmetry in these structures. Using Berry phase method we have calculated values of polarization and also reported electronic dielectric constant values.

MM 15.6 Mon 18:00 Poster E

Investigation of thermal properties of Si1-xGex melts under microgravity conditions — Bernd Damaschke[1], •Yuansu Luo[1], Suresh M. Chathoth[1], N.V. Abrosimov[2], M. Czupalla[2], and Korand Samwer[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Leibniz Institut für Kristallzüchtung Berlin

Investigation of thermal properties of Si1-xGex melts has been planned on board of the international space station (ISS) under microgravity and electromagnetic levitation (EML) conditions, where the absence of gravity-driven convection and segregation of the components allows precision measurements for the thermal expansion, surface tension and viscosity as function of temperature. The semiconductor alloy crystals for the ISS experiments were prepared by Czochralski growth. For the preparation, parabolic flights (PF), which provided a microgravity condition for ca. 20s, were carried out using the samples Si1-xGex made by arc-melting (x=0, 0.25, 0.5, 0.75 and 1.0). Preliminary data of their density, thermal expansion and surface tension in the melt and undercooled state were obtained. The density shows a non-ideal behavior with x and the highest value occurs at x=0.5, indicating a strong ordering tendency. We report about sample characterization and the status of the project concerning the ISS experiments. The initial results demonstrate that the melts of these alloys can be successfully processed in the MSL-EML facility for precision measurements on board the ISS. We thank DLR and Novespace for the PF campaigns and the MUSC team for the help with experiments. Financial support from DLR project 50WM0541 and 50WM1036 is gratefully acknowledged.

MM 15.7 Mon 18:00 Poster E

Molecular Dynamic Simulation of atomic deposition between MnAs cluster — •Andreas Rühl and Christian Heiliger — I. Physikalisches Institut, Justus Liebig Universtität Giessen, D-35392 Giessen, Germany

MnAs is a promising ferromagnetic material for magnetoelectronic devices, in particular as nano-scaled clusters, providing a great tunability concerning the shape and position. We investigate hexagonal MnAs clusters which are separated by a metal. Such structures could be produced by using a FIB (focused ion beam) two disconnect two touching MnAs clusters and to deposit a metal between them. Before doing a molecular dynamic simulation of the problem at hand one needs to find the corresponding effective potentials describing the interaction of the MnAs surface with the metal atoms. We did this by fitting the chosen potential model, here the Embedded Atom Method, to a set of ab initio data (Force Matching Method).

MM 15.8 Mon 18:00 Poster E

Ab initio calculation of phonon tunneling in Au/Vacuum/Au by atomistic Green's function formalism — •Saeideh Edalati Boostan, Michael Czerner, Michael Bachmann, and Christian Heiliger — 1I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Although phonons require matter to exist recent experimental and theoretical papers have shown that phonons can cross vacuum gaps of a few angstroms wide. This effect is called phonon tunneling [1,2,3]. In this work we calculate phonon tunneling in Au(111)/Vacuum/Au(111) by using an ab initio approach based on density functional theory. The interactions between atoms are modeled by inter atomic force constants, which are calculated by the abinit software package in the harmonic approximation. These inter atomic force constants are used as an input into an atomistic Green's function (AGF) method in order to calculate the transmission function of the system as a function of the thickness of the vacuum gap.

[1] Igor Altfeder et al., Phys. Rev. Lett. 105, 166101 (2010)
[2] Mika Prunnila and Johanna Meltaus, Phys. Rev. Lett. 105, 125501 (2010)
[3] D. P. Sellan et al., Phys. Rev. B 85, 024118 (2012)

MM 15.9 Mon 18:00 Poster E

Mechanical analysis of amorphous solids with large amplitude oscillatory spectroscopy (LAOS) — •Stefanie Finkhäuser, Carsten Mahn, and Konrad Samwer — 1.Physikalisches Institut, Georg-August Universität Göttingen

In the presence of mechanical fields glassy materials are known to reveal many interesting phenomena. One of them is a crossover from a linear behavior in stress-strain dependency to a nonlinear behavior. To investigate this crossover in detail we use dynamic mechanical excitation with large amplitudes and different frequencies. The sample is excited with a sinusoidal stress whose amplitude is large enough to lead to nonlinear strain-responses. The FFT-analysis of these nonlinear responses contains higher harmonic contributions. These can give further insight into interactions among local plastic events, which lead to the nonlinear response. We will show first results on PMMA and amorphous PdCuSi.

Financial support by the DFG SFB937 is thankfully acknowledged.

MM 15.10 Mon 18:00 Poster E

Charge and Spin transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweitzer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Jakoba Heidler[4], Xinliang Feng[3], Petr Ostrizek[1], and Mathias Kläui[1,2,4] — [1]4Institut für Physik, Johannes Gutenberg Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]FB Physik, Universität Konstanz, Universitätsstr. 10, D-78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, German — [4]SwissFEL, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Single Layer Graphene (SLG), which is a simple 2D honeycomb lattice made of carbon atoms, is still one of the most promising materials for scientific research and moreover for nanoelectronic and spintronic devices. Here we present electrical and magnetic transport in two highly interesting Graphene allotropes: Turbostratic Graphene (TG) and Graphene Nanoribbons (GNR). TG is a stack of Graphene where every layer is rotated by a certain angle. Nevertheless it retains important properties similar to SLG due to electronical decoupling. High mobilities of 10^5 cm^2/Vs were measured in TG discs [1] and spin injection in a non-local spin valve [2] has been investigated. Measurements with atomically precise GNR [3] indicate quantum transport behaviour at low temperatures and theory predicts magnetic edge states [4].

[1] Y. Hernandez et al., (under review). [2] N. Tombros et al., Nature 448, 571 (2007). [3] Cai et al., Nature 466, 470-473 (2010). [4] O. Yazyev et al., Phys. Rev. Lett. 100, 047209 (2008)

MM 15.11 Mon 18:00 Poster E

Stability Analysis of Intrinsic Colloidal Quasicrystals: A Recipe for Designing Quasicrystals — •Erdal Celal Oğuz and Michael Schmiedeberg — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

A big advantage of studying colloidal quasicrystals is that individual particle positions are directly observable (eg. by using video-microscopy) and therefore real-space information is accessible. Another advantage is that the interaction between the colloidal particles in principle can be fine-tuned. In this work, we investigate the ground state (T=0) stability of colloidal quasicrystals by minimizing the lattice sum. For this purpose, we develop lattice summation techniques for quasicrystals with 5-, 8-, 10- and 12-fold rotational symmetry. Subsequently, we minimize the potential energy with respect to particle coordinates for various pair interaction potentials with two length scales. Our goal is to find suitable isotropic interaction potentials that lead to stable quasicrystalline order.

MM 15.12 Mon 18:00 Poster E

Symmetry and electronic structure study of a predicted carbon structure — •Torsten Weissbach, Silvia Bahmann, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

A new metastable structure for carbon, which is presented in by the authors in another contribution, was predicted theoretically. It consists of structural building blocks of diamond and graphite and exhibits tubular pores, similar to the carbon foam class of structures. Here, we investigate the symmetry of the structure and its reflection in the calculated electron and phonon band structure. Like graphite, this new carbon structure exhibits a band crossing at the Fermi level and zero band-gap. Compared to graphite, the deformation stability is enhanced by the links between the graphene planes.

MM 15.13 Mon 18:00 Poster E

Characterization of Pulsed CNT Field Emitters for Medical Imaging — •Daniela Leberl[1,2], Bernhard Hensel[2], and Sandro Francesco Tedde[1] — [1]Siemens AG, Corporate Technology, Erlangen, Germany — [2]Center for Medical Physics and Engineering, University Erlangen-Nuremberg, Erlangen, Germany

Cold electron sources for X-ray applications would be beneficial for reduced acquisition time and improved image quality compared to thermionic emitters, today's state of the art. Carbon nanotubes (CNTs) are a promising material for field emission applications due to the high aspect ratio and high electrical and thermal conductivity. For motion-free 3D image acquisition, short electron pulses of many individual sources are necessary. Thus it is important to investigate the field emitter characteristics and stability under pulsed conditions.

Here we report on electrical characterization of multi-walled CNTs grown by thermal chemical vapour deposition on stainless steel substrates. We studied the dependence of the IV characteristics and emitter stability on pressure, pulse-on time and duty cycle. All investigations have been carried out on samples with high field emission currents up to 126 mA (220 mA/cm^2) and extremely long lifetimes up to 200 cumulative hours.

We found out that the emitter degradation is an important parameter for the application in medical X-ray systems. We discuss potential degradation mechanisms and present the correlation with threshold field and field enhancement factor, calculated with the Fowler-Nordheim theory of field emission.

MM 15.14 Mon 18:00 Poster E

Stacking faults in fcc Iron: The Influence of Magnetism — •Ivan Bleskov, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

The stacking fault energy is a critical parameter that defines the type of plasticity mechanism in austenitic high-Mn steels, which are char-

acterized by a combination of enhanced formability and strength. A common concept for its description is the generalized stacking fault energy (γ-) surface, which describes the sliding of one part of a perfect crystal against the other. It provides the energy paths and barriers, which the system needs to overcome to form an intrinsic stacking fault (ISF). The goal of the present work is to study the influence of magnetism on the topology of the γ-surface. To avoid the influence of chemical effects, we have focused the investigation on pure fcc Fe. Density functional theory has been used for calculations of different magnetic (non-, ferro- antiferro-, and paramagnetic) structures. The paramagnetic state, which is closest to reality, was approximated by the disordered local moments (DLM) realized within the coherent potential approximation. Changing to magnetically ordered structures the γ-surface is strongly altered. The effects are stronger for ferro- than for antiferromagnetic configurations. The nonmagnetic γ-surface, however, is in the relevant region in very good agreement with DLM, and therefore may be used to reduce the complexity in future ISF calculations.

MM 15.15 Mon 18:00 Poster E

Investigation of the loading state dependent fracture behaviour of nanocrystalline PdAu — •Christian Braun and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

Numerous experiments exhibited that nanocrystalline materials with a mean grain size in the range of 10 to 20 nm behave different in compression and tension testing, in agreement with molecular dynamic simulations. However, investigations with other loading conditions between these two limiting cases are still scarce.

We used the miniaturized shear compression specimen (m-SCS) to study the mechanical response of nanocrystalline PdAu samples under different loading states by varying the shear angle. Since the deformation of the m-SCS samples is constrained to a cross section of 0.1 mm^2, it becomes possible to in-situ observe plastic shear and/or crack nucleation and propagation using light microscopy. Additional, post mortem REM-analysis of the fracture surfaces is carried out. We present results for specimens with shear angles of 45° and 60°. Although, upon loading a specimen, the difference in the hydrostatic pressure is small between this two sample geometries, they show a completely different behaviour: while for the 45° specimens a ductile deformation up to 20% strain is observed, the 60°-samples show brittle fracture in the transition regime from elastic to plastic deformation.

MM 15.16 Mon 18:00 Poster E

Shear compression specimens - a new approach to study the pressure and normal stress dependence of plasticity — •Christian Braun, Patrick Marx, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

The mechanical behaviour of several materials which are currently in the focus of research, like nanocrystalline metals or metallic glasses, exhibits a compression-tension-asymmetry, i.e. yielding depends on the loading condition. While this compression-tension-asymmetry of yielding is well examined in simulations, experiments are still rare for various reasons: On the one hand the ductility of these materials is often limited in a tensile test and on the other hand there are only a few involved methods to probe other loading states than pure compression and tension.

A new approach to study the pressure or normal stress dependence of plasticity is exploiting shear compression specimens (SCS) with different shear angles. The sophisticated data analysis of these experiments based on FEM-simulations allows to extract all components of the stress and strain tensor and so to relate the state of stress to the observed yielding behaviour. We present a feasibility study with stainless steel as reference material to demonstrate the potential of this testing method.

MM 15.17 Mon 18:00 Poster E

Relationship between enthalpy relaxation and shear modulus relaxation below and above the glass transition of metallic glasses — •Yuriy Mitrofanov[1,2], Andrey Makarov[3], Vitaly Khonik[3], Andrew Granato[4], Dave Joncich[4], and Svetlana Khonik[5] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Solid State Physics, State Technical University, Voronezh, Russia — [3]Department of General Physics, State Pedagogical University, Voronezh, Russia — [4]Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA — [5]Centre for Joint Research, State University, Voronezh, Russia

Despite decades-long investigations of the enthalpy relaxation in metallic glasses, its nature remains unclear. To understand the nature of the enthalpy relaxation near Tg, we used an approach, that is based on the interstitialcy theory. We derived a simple and testable expression for the heat flow (enthalpy relaxation rate) occurring upon heating of the glass at a constant rate. This heat flow is mostly determined by the shear moduli of the glass and the parent crystal. The shear modulus of the glass is defined by the concentration of frozen-in interstitialcy-like defects (atomic configurations with two atoms sharing the same potential well). The relaxation law describes both, the exothermic heat flow below Tg and endothermal heat flow above Tg and reflects a generic connection between the elastic properties of the glass and the parent crystal. An extensive check of the derived heat flow law for temperatures near the glass transition showed good agreement with the experiments performed on two Pd-based metallic glasses.

MM 15.18 Mon 18:00 Poster E

Time dependent development of decorated grain boundaries of severely plastically deformed Al by liquid Ga — •mehrnoosh naderi, martin peterlechner, gerhard wilde, and sergiy divinskiy — Institute of Material Physics, University of Muenster, Germany

Fast liquid penetration into the grain boundary network of a polycrystalline solid is observed for different metallic or ceramic couples. Yet, the detailed mechanism as well as morphological features or the kinetics of the penetration process are not well understood. Recent models relate the liquid penetration process to the mechanical properties of the grain boundaries. In order to investigate the importance of defect structures and residual stresses at grain boundaries for the liquid penetration kinetics, the penetration behavior of liquid Ga along fine grains of polycrystalline Aluminum produced by High Pressure Torsion was studied at room temperature. Scanning Electron Microscopy (SEM) and the so-called Automated Crystal Orientation Mapping (ACOM) technique that measures the orientations in a transmission electron microscope (TEM) have been used for this study. The development of decorated grain boundaries was investigated by SEM and the thickness of Ga layer at grain boundaries was obtained less than 1.5 nm from ACOM data as well. The results are discussed with respect of the underlying mechanism that drives liquid penetration into the grain boundary network.

MM 15.19 Mon 18:00 Poster E

Rational Tuning and Thermodynamic Characterization of Lithium Silicides as Electrode Materials for Lithium Ion Batteries — •Thomas Gruber and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics,Leipziger Str. 23, 09596 Freiberg, Germany

Li_xSi is a promising anode material for lithium ion batteries due to its high specific energy density. There are several known stable phases with different Li/Si ratio. The main goal of our investigation is to support an understanding of the charging and discharging processes, which are directly related to the Li^+ transport. For practical usage of Li_xSi in lithium ion batteries a proper understanding of the thermodynamical behavior of the material is required. The Gibbs free energy can be determined from the calculation of the phonon dispersion, which depends on pressure. We have calculated the isotropic thermal expansion of Li_7Si_3 and the non-isotropic thermal expansion of LiSi. This gives access to the thermal expansion coefficients, speci*c heat and other thermodynamical data. Our theoretical results are then compared to experimental data measured on these compounds.

MM 15.20 Mon 18:00 Poster E

Understanding the protein-inorganic crystal interaction in bioinspired syntheses — •Annalena Wolff[1], Idir Yahiatene[1], Walid Hetaba[2], Nadine Mill[1], Marco Wissbrock[3], Stefan Loeffler[2], Katrin Eckstädt[1], Norbert Sewald[3], Peter Schattschneider[4], and Andreas Hütten[1] — [1]Uni Bielefeld, Fakultät für Physik — [2]TU Wien, Institut für Festkörperphysik — [3]Uni Bielefeld, Fakultät für Chemie — [4]TU Wien, Service Center für Elektronenmikroskopie

Bioinspired syntheses have sparked great interest in the past years. Recent studies showed that proteins, involved in nanoparticle formation within natural systems, can be used to influence materials, not known to occur within these systems. The engineering process however remained elusive. Here, cobalt ferrite nanoparticles were synthesized using c25-mms6, a short synthetic version of a protein linked

to nanoparticle formation in magnetotactic bacteria. The polypeptide allows the formation of stoichiometric, shape specific nanoparticles, which cannot be achieved under similar conditions by conventional chemical synthesis. The particles were studied at different times during nanoparticle growth using TEM, HRTEM and EELS to gain a better understanding of the engineering process. The polypeptide - inorganic crystal interaction was studied in FCS measurements. The results suggest that the polypeptide adsorbes onto the (111) face of the particles,reduces its surface energy, and allows the formation of hexagonally shaped nanoparticles. The polypeptides can be easily removed after the growth process which is advantageous for applications.

MM 15.21 Mon 18:00 Poster E

Influence of the sputter parameters on surface segregation and silver ion release properties of reactively sputtered Ag/TiOx nanocomposites — •Jian Xiong[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Ulrich Schürmann[2], Lorenz Kienle[2], Frank Lehmann[3], and Franz Faupel[1] — [1]Institute for Materials Science-Multicomponents Materials, CAU Kiel, Kaiserstr. 2, 24143, Kiel, Germany — [2]Institute for Materials Science- Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143, Kiel, Germany — [3]Dept. of Prosthodontics, Propaedeutics and Dental Materials, CAU Kiel , Arnold-Heller-Str. 3, 24105, Kiel, Germany

Reactive sputtering of silver/titania nanocomposites is potentially attractive for antibacterial coatings based on the release of silver ions. Previous studies on such coatings showed strong segregation of silver towards the surface. Surface segregation leads to rapid depletion of the Ag in humid invironment and prevents tailoring of the release properties. In this work, the influence of sputter parameters on the morphology and subsequent silver ion release properties of reactively sputtered silver/ TiOx nanocomposites was investigated. It was observed that silver surface segregation is largely independent of the oxygen partial pressure used in the sputtering process and that - unlike in nonreactive sputtering of TiOx - even sputtering of pure TiOx barriers at moderate deposition rates is not sufficient to prevent the strong surface segregation. Surface segregation is significantly reduced for silver filling factors below a critical silver content of 9% and can be further be reduced by deposition of TiOx barriers with high sputtering rates.

MM 15.22 Mon 18:00 Poster E

Influence of transition-metal alloying on the electro-chemical properties of (Li)$FePO_4$ as cathode material for Li-ion batteries — •Hamid Reza Hajiyani, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

One of the central challenges in increasing the performance of Li-ion batteries is the optimization of cathode aterials. The candidate compounds need to provide a technologically acceptable compromise of energy density, intercalation voltage, as well as structural and thermal stability during intercalation. A promising approach to achieve this goal for cathode materials based on $FePO_4$ is alloying by partly or fully substituting Fe with other transition metals (TMs). Here, we use high-throughput density-functional theory (DFT) calculations in order to investigate $LiM_yN_{(1-y)}PO_4$ compounds in the olivine structure. In particular, we determine the formation energy for various stoichiometric of different TMs M and N. Systematic screening across the 3d TM allows us to identify alloying trends with bandfilling and atomic size. For each binary TM phosphate we consider different levels of Li intercalation. Based on these DFT calculations we estimate the energy density, the volume expansion during intercalation, the intercalation voltage, and the thermal stability with respect to oxidation. Our calculations indicate that the energy density of the binary transition metal phosphates increase with bandfilling while the thermal stability of the compounds decreases.

MM 15.23 Mon 18:00 Poster E

Cluster expansion study of Ni–Pt alloys — •Martin Leitner, David Reith, and Raimund Podloucky — Department of Physical Chemistry, University of Vienna

The Cluster expansion (CE) is a state-of-the-art tool for exploring the configuration space of multi-component systems with the accuracy of density functional theory (DFT) calculations. Based on the figure set of a converged CE Monte-Carlo (MC) simulations are performed in order to derive temperature dependent phase stabilities.

This CE+MC approach – as implemented in the UNCLE package [1] – is applied to study the Ni–Pt alloy system, for which the formation of ordered phases at low temperatures is under debate. DFT studies focussed on three ordered phases, namely $NiPt_3$ and Ni_3Pt with $L1_2$ structure and NiPt with $L1_0$ structure. A CE study predicted an additional stable Pt-rich phase of $NiPt_7$ composition, which was not confirmed by recent DFT studies and experiment. A further DFT study predicted a Ni-rich Ni_3Pt phase with $D0_{22}$ ordering to be energetically more favorable than the $L1_2$ structure.

Based on DFT calculations performed with VASP an extensive CE+MC study was done for the whole composition range. The results will be critically compared to the existing data. Furthermore, calculated short range order intensities are compared to very recent X-ray Photon Correlation Spectroscopy (XPCS) experiments in the Ni-rich regime.

Supported by FWF, project nr. F4110 (ViCoM).

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

MM 15.24 Mon 18:00 Poster E

DFT studies of the lattice thermal conductivity of thermoelectric materials — •René Moser[1], Mingxing Chen[2], and Raimund Podloucky[1] — [1]Department of Physical Chemistry, University of Vienna — [2]Department of Physics, University of Wisconsin-Milwaukee

Thermoelectric materials are of technological and scientific interest because of their ability to convert a temperature gradient directly into electric energy. The efficiency of this process is defined by the figure-of-merit $Z = TS^2\sigma/\kappa$ which contains the Seebeck coefficient S, the electrical conductivity σ and the thermal conductivity κ at a given temperature T. A large Z is achieved by a large S and a small κ, which properties one tries to optimize. The total thermal conductivity $\kappa = \kappa_{el} + \kappa_{ph}$ is the sum of the electronic contribution κ_{el} and the phonon mediated lattice thermal conductivity κ_{ph}. Here we focus on the first-principles modelling of κ_{ph} by a density functional (DFT) theory approach for the electronic structure and phonon properties in combination with Boltzmann's transport theory. Results are presented and discussed for a selection of thermoelectric materials.

Supported by FWF, project nr. P24380.

MM 15.25 Mon 18:00 Poster E

Matrix-induced in situ growth of plasmonic Au nanoparticles for biological sensor devices — •Philipp Naujok[1], Christian Katzer[1], Peter Michalowski[1], Frank Schmidl[1], Markus Westerhausen[1], Gabriele Schmidl[2], Robert Mueller[2], Jan Dellith[2], Christa Schmidt[2], Jacqueline Jatschka[2], and Wolfgang Fritzsche[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena - Helmholzweg 5, D-07743 Jena, Germany — [2]Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, D-07745 Jena, Germany

In the past years different methods such as wet chemical synthesis where established to fabricate metal nanoparticles which can be used in bio-photonic sensor devices. In order to overcome the multiple preparation steps and typical solution based problems like aggregation of particles, new in-situ methods of preparation directly on the substrate surface are highly favoured. The authors present a novel in-situ method of fabricating crystalline gold nanoparticles by self-organization using two different thin film matrices ($YBa_2Cu_3O_{7-\delta}$ and $SrTiO_3$). We will show that the interaction of nanoparticles and thin film matrix allows controlling not only the size (between 10 and several hundreds of nm) and distribution of gold nanoparticles but also their shape. A subsequent dissolution process of the matrix enables us to extract the nanoparticles to receive immobilized crystalline particles directly on a substrate surface. The spectral characterization of those particles will be presented based on microspectroscopy. [1] C. Katzer et al., J. Nanopart. Res. 14, 1285 (2012)

MM 15.26 Mon 18:00 Poster E

Coulomb drag in monolayer graphene — •Jonathan Lux — Institut für theoretische Physik, Universität zu Köln

Coulomb drag measurements provide an interesting possibility to study interaction effects between two adjacent layers. If a current is driven in one of the layers, called the active layer, via Coulomb interaction, momentum can be transferred to the other layer, called the passive layer. This can induce a voltage drop in the passive layer, which can be measured. The ratio of the voltage drop in the passive layer and the current in the active layer is called the drag resistance.

We have calculated the drag resistivity in MLG using Boltzmann kinetic theory, taking into the two relevant modes for both particles and holes in each layer. In the Fermi liquid (FL) regime of monolayer graphene (MLG), the drag resistivity is, up to numerical prefactors,

identical to the one in the 2 dimensional electron gas, and independent of the impurity configuration.

Near charge neutrality, Coulomb interaction is able to relax the current, due to the particle–hole symmetry of the low energy Dirac theory of MLG. This defines a new regime, which is not accessible in FLs. We found that here the result depends on the ratio of the scattering times of Coulomb and impurity scattering. In the very clean limit, when the impurity density reaches zero, the drag resistivity assumes an universal finite value, although the individual conductivities diverge.

MM 15.27 Mon 18:00 Poster E

Stacking fault energy of a binary Fe_xMn_{1-x} mixed crystal calculated by combing cluster expansion and DFT — •Sebastian Schwalbe, Torsten Weissbach, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

Physical properties like mechanical stability and ductility of highly alloyed steels play an important role in material science. The stacking fault energy (SFE) [1] is a powerful instrument for the characterization of such systems. Both cluster expansion (CE)[2] and the calculation of the SFE can be expressed with the Ising-model formalism. The CE relies on the division of the lattice into different geometrical clusters, and calculating their total energy (e.g. using LAPW[3]). This enables the calculation of total energies for mixed crystal models. The aim of this work is to exploit the combination of DFT and CE for the special case of SFE computation.

[1] Vitos,L., Nilsson, J.-O. & Johansson, B.: Acta Materialia (2006), 54, 3821-3826.
[2] A. van de Walle: Calphad Journal (2009), 33, 266.
[3] Blaha, P.,Schwarz, K., Madsen, G. K. H., Kvasnicka, D., Luitz, J.: WIEN2k, Techn. Universität Wien, Austria, 2001.

MM 15.28 Mon 18:00 Poster E

Investigation of possible solid state reaction in the Fe-Al-O system based on density functional theory. — •Lilit Amirkhanyan, Torsten Weissbach, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

Particles in a metallic melt can be filtered out using ceramic filters, which are often based on corundum. From experiments it is known that new phases (e.g. $FeAl_2O_4$) can be formed during the filtering process. We study several solid state reactions using density functional theory (DFT) calculations. By varying the volume and calculating the corresponding total energy we obtained the equation of states for α-Al_2O_3, metastable κ-Al_2O_3, Fe_2AlO_4, $FeAl_2O_4$, $FeAlO_3$, FeO.

This allows to discuss possible phase formation mechanisms based on energy differences obtained from DFT. In particular we will focus on the possibility to form hercynite $FeAl_2O_4$.

MM 15.29 Mon 18:00 Poster E

High Throughput Preparation and Scanning of a Complex Perovskite Oxide Library for Light-driven Electrocatalysis — •Helge Stein, Andreas Blumenstein, Julius Scholz, Jörg Hoffmann, and Christian Jooss — Institut für Materialphysik, Friedrich-Hund Platz 1 37077 Göttingen, Deutschland

With respect to development of novel materials for sunlight driven photocatalysis, high-throughput preparation and characterization methods are preferable because of the broad chemical search space. We have designed a system for the screening and production of ternary and quaternary oxide compounds in order to find promising compositions which have a well-matched electronic band structure and sufficient complexity to enable a multi-step charge transfer reaction. As a model system we have prepared a multi-component La-Sr-Fe-Co (LSFC) oxide library for testing oxygen evolution under sunlight irradiation. This system is mostly of perovskite type and shows a broad doping ability as well as a complex electronic structure. The samples were deposited on glass using an ink-jet printing technique with nitrate precursors. By post-annealing in air for 4 hours at 480°C Oxide phase formation was performed. Electrocatalytic measurements were made by high throughput cyclic voltametry in darkness and under illumination. The Crystallographic structure and surface morphology of the samples was determined by x-ray and SEM techniques.

MM 15.30 Mon 18:00 Poster E

Grain boundary free energies from the reweighted path ensemble — •Jutta Rogal and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The grain boundary free energy and mobility are important quantities in describing grain growth and thus the evolution of the microstructure in polycrystalline materials. In this study we use transition path sampling (TPS) to investigate the transformation of one particular grain orientation into another via the migration of a grain boundary within a Lennard-Jones system. The trajectories describe the entire transition including the initial formation of the grain boundary. By reweighting the path ensemble it is then possible to extract the free energy as a function of any arbitrary order parameter and thus determine the grain boundary free energy at various temperatures. Since all trajectories in the path ensemble are true dynamical trajectories of the system the path ensemble also contains information about the mobility as well as the migration mechanism of the grain boundary.

MM 15.31 Mon 18:00 Poster E

High-Performance LFP Thin Film Electrodes — •Frank Berkemeier, Mathias Köhler, Lea Lüken, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm Str. 10, D-48149 Münster

Thin films of lithium iron phosphate (LFP) are prepared by reactive ion beam sputtering, with a thickness between 50 and 500 nm. The structure and morphology of the layers is investigated by X-ray diffraction measurements and transmission electron microscopy, while their electrochemical properties are characterized by means of cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and the galvanostatic intermittent titration technique (GITT). It is observed that the electrochemical performance of the layers strongly depends on the preparation conditions during sputtering. Thus, using optimum deposition conditions, a reversible capacity of 104 $mAh\,g^{-1}$ is found, and a cycling stability at 1 C rate which allows to perform more than 1700 cycles before observing a capacity loss of only 20%. In addition, the lithium diffusivity is measured by EIS and GITT, and is found to be in the range of 10^{-13} cm^2s^{-1}. This quite high diffusivity value is attributed to the strong texture of the deposited LFP films.

MM 15.32 Mon 18:00 Poster E

V_2O_5 thin films for Li-ion battery applications — •Tobias Gallasch, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Ion beam sputtered V_2O_5 thin films (thickness 10 nm - 200 nm) are investigated electrochemically via cyclic voltammetry and chronopotentiometric measurements. Within these measurements a capacity of about 400 mAh/g for reversible lithium storage is reached. In addition, Li^+ diffusion coefficients are determined by different approaches and compared to each other.

Structural changes between as-prepared, partially charged and cycled thin films are evaluated in detail by HR-TEM and EELS and the lithium signal is evaluated, directly, depending on the state of charge.

Thus, in this work the link between Li intercalation processes and morphological changes is worked out combining modern techniques of electrochemistry and analytical TEM.

MM 15.33 Mon 18:00 Poster E

Percolated Pd thin films for hydrogen sensors — •Magnus Hamm, Stefan Wagner, and Astrid Pundt — Institut für Materialphysik, Friedrich-Hundt-Platz 1, D-37077, Goettingen, Germany

It's easy accessibility and high chemical energy density makes hydrogen interesting as a future energy carrier. In addition hydrogen allows a CO2 free energy production by its reaction with oxygen to water. However one major drawback of hydrogen is its dangers when in contact with oxygen. At concentrations in the regime of 4% to 94% hydrogen is highly flammable and explosive, which makes it difficult to store and transport. Out of these reasons effective hydrogen sensors are needed for a large scale hydrogen energy network. In this work the up-to-date development of hydrogen sensors is presented and compared to a new type of thin film palladium sensor. We deposited thin Palladium films on Sapphire substrates. Later the film was fractured by Joule heating. This leads to a percolated surface which shows large resistivity effects when contacted with hydrogen. The Sensor shows good reversibility at slow reaction and decay times in the minute range. However the resistivity changes up to 6000% when contacted with hydrogen and the minimal detection limit lies at 10-20 mbar, values which both exceed other hydrogen sensors. Financial support by the DFG via PU131/9 and SFB602 is gratefully acknowledged.

MM 15.34 Mon 18:00 Poster E

Electrochemical Hydrogenography of Palladium, Magnesium

and Titanium — •Jara Kürschner and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Germany

The storage of hydrogen in metals is a safe and volumetrically desirable way. Rapid determination of the hydrogen concentration c_H in gas-phase loaded metal thin films can either be done by resistivity or transmission measurements as the electronic structure of the metal changes during hydrogenation. Since some years, the optical transmission T is applied in a technique named "Hydrogenography" to determine the hydrogen concentration in thin alloy films. A linear relationship $c_H \propto \ln(T/T_{Metal})$, as predicted by the Lambert-Beer law, is commonly assumed although it holds the assumption of the free lattice gas model.

The model does neither imply non-homogeneous hydrogen distributions as occurring during phase transitions of many metal-hydrogen systems, nor stresses, plastic deformation and film buckling which are often arising in clamped thin films.

This study analyzes the dependency between optical transmission and hydrogen concentration for clamped and quasi-free palladium, magnesium and titanium thin films. Via electrochemical hydrogen loading, the hydrogen concentration is independently controlled and the applicability of the Lambert-Beer law can be tested.

Financial support by the DFG via PU131/9 and PU131/10 is gratefully acknowledged.

MM 15.35 Mon 18:00 Poster E

Influence of hydrogen on Ta(110) surfaces — •Sebastian Schleicher, Sara Wanjelik, and Mathias Getzlaff — Heinrich-Heine-Universität

Hydrogen in metals has attracted a lot of attention in the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamental point of view.The goal of our investigations is a study of hydrogen absorbtion in a Ta(110) crystal. Careful cleaning of the Tantalum surface is essential as preparation for any measurement. The cleaning procedures are similar to those already discussed in various publications, involving flashing to high temperatures close to the melting point to remove H and O absorbates, and heating in an oxygen atmosphere to remove residual carbon impurities. Measurements are performed by means of scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) in ultra-high vacuum conditions.

MM 15.36 Mon 18:00 Poster E

Second-Harmonic Generation in Silver Nanorod Arrays — •Fabian Patrovsky[1], Vera Hoffmann[1], Philipp Reichenbach[1], Andreas Hille[1], René Kullock[2], and Lukas M. Eng[1] — [1]Institute of Applied Photophysics, TU Dresden, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Germany

Second-harmonic generation (SHG) in metal nanoparticles is a promising new field combining nanotechnology with nanooptics [1]. Previous studies excellently proved the SHG effect of single nanoparticles attached preferentially to nonconductive surfaces. Similar to Raman scattering [2], the SHG efficiency can be considerably increased when coupling two such nanoantennas in the optical near-field region [3].
In the present study we investigate the generation of second-harmonic radiation from silver nanorod arrays as a function of different geometric parameters (volume, rod length, distance) including also the angle of incidence. Correlations between linear and nonlinear optical properties are found.

[1] M. D. McMahon et. al. Physical Review B 73, 041401(R) (2006) [2] P. Olk et. al. Nano Lett. 7 (6), pp 1736-1740 (2007) [3] R. Jin et. al. J. Am. Chem. Soc. 127, 12482 (2005)

MM 15.37 Mon 18:00 Poster E

Electric field gradient at the A site in selected MAX phase solid solutions studied with perturbed γ-γ angular correlation — •Christoph Brüsewitz[1], Daniel Jürgens[1], Ulrich Vetter[1], Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

MAX phases represent a class of complex carbides and nitrides which combine prominent features of both metals and high performance ceramics. They are good electric and thermal conductors, thermal and mechanical shock resistant, and easily machinable. Perturbed γ-γ angular correlation (PAC) offers, using implanted ^{111}In as probe atom, an insight into the local environment of the probes at the A-sites of many MAX phases by studying the electric field gradient (EFG). Starting with Ti_2AlC, the variation of the EFG caused by systematic replacement of half of M atoms with V, A atoms with In, and X atoms with N is investigated. Additionally, these results are compared with the EFG of the corresponding end members V_2AlC, Ti_2InC, and Ti_2AlN. The existence of a single phase is confirmed through XRD. This work is supported by the DFG under contract HO 1125/19-2.

MM 15.38 Mon 18:00 Poster E

Electrochemical lithiation/delithiation analysis of silicon as anode material for lithium-ion batteries — •Gibaek Lee[1,2], Stefan L. Schweizer[2], and Ralf B. Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials — [2]Martin-Luther-University Halle-Wittenberg

It has been known for some time that silicon can incorporate large amounts of Li with a specific capacity of 4200 mAh/g, about a factor of 11 larger than for state of the art graphite anodes. However, silicon and silicon-based negative electrodes exhibit huge volume expansion (ca. 270%) during lithiation/delithiation, resulting in mechanical disintegration of electrode and rapid capacity fading. Therefore, relaxation of the stress caused by the expansion and contraction of Li-Si alloy materials is important to obtain a good cyclability.

In this study, we prepared oriented silicon nanowire arrays (SiNWs) on n-type silicon substrate by metal-assisted chemical etching in aqueous HF solution containing AgNO3. The electrochemical properties of the SiNWs electrode were systematically investigated. The material characteristics have been analyzed by Cyclic voltammetry (CV), XRD, SEM and TEM. The performance of SiNWs electrode have been examined by galvanostatic charge/discharge cycling. In addition, to compare the battery cycle behavior of the different structure of silicon anode material, we have investigated the characteristic and transformation of other types silicon anode such as black silicon and macroporous silicon obtained by reactive ion etching (RIE) etching and electrochemical etching, respectively.

MM 15.39 Mon 18:00 Poster E

Phase-field crystal approach to model interfaces and crystal nucleation in binary alloys — •Muhammad Ajmal Choudhary[1], Julia Kundin[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth. — [2]Institut für Angewandte Physik, Universität Tübingen, D-72076, Tübingen.

In general, the properties of a material are strongly related to the nucleation and patterning of its microstructure. Phase-field crystal (PFC) modeling is widely used to address the nucleation and microstructure evolution phenomena. We used a binary alloy system to study the equilibrium properties of liquid-solid interfaces as well as the nucleation barriers. We proposed the method of determining interfacial energies for a curved liquid-solid interface by stabilizing the circular solid seed in the surrounding liquid phase as well as the liquid droplet in the solid phase for various seed sizes in a finite system. We also derived the free energy barriers for the nucleation and investigated the system size effects on the equilibrium properties of liquid-solid interface and nucleation barriers. Furthermore, we compared the simulation results with the existing theories as well as the predictions based on the classical nucleation theory.

MM 15.40 Mon 18:00 Poster E

DFT calculation of cleavage energies and γ-surfaces in Mo_2BC hard coatings — •Tobias Klöffel[1], Sandra Korte[2], and Bernd Meyer[1] — [1]Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg — [2]Lehrstuhl für Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg

The unusual combination of high stiffness and moderate ductility makes Mo_2BC a very interesting material for application as hard protective coating of cutting tools. In order to obtain more detailed insights into the properties of dislocations and plastic deformation in Mo_2BC we have calculated the γ-surfaces for several crystallographic crystal cuts using density functional theory. For many simple fcc and bcc metals a detailed atomistic understanding of dislocation properties has been gained on the basis of Peierls-Nabarro models and calculated γ-surfaces. However, such an approach has not been attempted yet for more complex compounds such as Mo_2BC. Here, the first results on the shape and properties of the γ-surfaces will be discussed. It will

be shown that it is not possible to conclude from the decohesion energy which crystallographic plane will be the active plane for plastic deformation. Finally, the results for the critical Peierls stress and the preferred shear planes will be compared to experimental observations in mechanical tests on micrometer-sized Mo_2BC pillars.

MM 15.41 Mon 18:00 Poster E

First-principles calculations and kinetic Monte Carlo simulations of screw dislocation motion in dilute W alloys — •Leili Gharaee[1], Alexander Stukowski[2], Jaime Marian[3], and Paul Erhart[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Lawrence Livermore National Laboratory, Livermore, California

Tungsten is being considered as a candidate material for structural applications in fusion reactors. The performance of the pure material is, however, limited by a high ductile-to-brittle transition temperature (DBTT), which can be lowered by alloying for example with small amounts of Re. These alloys are, however, not suitable for applications in fusion environments due to neutron activation of Re, which motivates the search for alternative alloys. The present work addresses the potential of dilute W-Ti alloys to accomplish a lowering of the DBTT. To this end, we have studied the elastic properties of intrinsic defects and substitutional alloying agents in body-centered cubic tungsten as well as their direct interaction with screw dislocations using density functional theory. In this fashion we determined deformation volume tensors and interaction strenghts for each of these entities. The thus obtained information was subsequently employed to parametrize a kinetic Monte Carlo model for screw dislocation motion that takes into account the elastic interaction between dislocation segments and point defects. This approach enabled us to study systematically the effect of various defects on the mobility of screw dislocations as a function of shear, temperature, and defect density.

MM 15.42 Mon 18:00 Poster E

Highly ordered metal nanowire arrays as active substrate of SERS — •Yong-Tae Kim[1], Stefan L. Schweizer[1], and Ralf. B. Wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg — [2]Fraunhofer Institute for Mechanics of Materials

Metallic nanostructured materials have fascinating potential applications in the nanodevices, especially as an efficient substrate for surface-enhanced Raman scattering (SERS). In SERS, as one of the most promising optical sensing techniques, the Raman signal can be amplified by several orders of magnitude by the use of metallic nanostructure substrates. 1-dimensional metallic nanostructures show some advantages associated with their anisotropic architecture and enable to be employed as highly active substrate of SERS.

The key obstacle for the practical use of SERS devices is the lack of robust and facile fabrication strategies for reproducible SERS substrates with stable enhancement. Although traditional SERS substrates such as colloidal nanoparticles, metal islands, and fractal film provide significant SERS enhancement, the well ordered 1-dimensional metallic SERS substrates with reproducible and deterministic geometries are needed for detection of trace level molecules in gases or liquids.

In this study, single- or multi-segmented 1-dimensional highly ordered metallic nanowire arrays composed of nickel, silver, and gold have been fabricated by simple pulsed electrodeposition in the pores of anodic aluminum oxide (AAO). Various 1-dimensional metallic nanowire arrays with different diameter, length, and sequence of metal segments are tailored as active substrate of SERS.

MM 15.43 Mon 18:00 Poster E

Auf $Pt/peO - TiO_2/Ti$ **basierender** H_2**-Generator** — •Ömer Cakabay, Mhamed El Achhab und Klaus Schierbaum — Heinrich-Heine-Universität Düsseldorf, Institut für Experimentelle Physik der kondensierten Materie, Abteilung für Materialwissenschaft, Universitätsstraße 1, 40225 Düsseldorf

Wir berichten über die Entstehung einer elektromotorischen Kraft an Platin-bedeckten plasmaelektrolytisch oxidierten Titanfolien, die bei Raumtemperatur von einem Wasserstoff-Sauerstoff-Gemisch beströmt werden [1]. Bei diesen Bedingungen kann man entweder eine Spannung $V \leq 465$ mV zwischen Platin und Titanfolie messen, wobei der Platinkontakt gegenüber dem Titankontakt positiv ist, oder einen Kurzschlußstrom; wir haben Proben hergestellt, bei der die Kurzschlußstromdichte Werte von bis zu 20 mA/cm^2 aufweisen kann, wenn der Wasserstoffgehalt 3,5 Vol-% in Luft beträgt und die Probe in einer Stömungsapparatur mit einem Gasstrom von 100 ml/min überströmt wird. Stromabwärts beobachtet man eine Verringerung der Wasserstoffkonzentration und eine Erhöhung der Feuchtekonzentration, die die katalytische Oxidation von H_2 am Platin beweist. In dem Beitrag werden diese Messungen quantitativ ausgewertet; sie bestätigen auch das einfache physikalisch-chemische Modell dieses Chemogenerators, das in [1] vorgeschlagen wurde. Wir berichten auch über präparative Möglichkeiten zur Erhöhung der Stromdichte dieses Chemogenerators.

[1] K. Schierbaum and M. El Achhab, Phys. Status Solidi A 208, No. 12, 2796-2802 (2011) / DOI 10.1002/pssa.201127400

MM 15.44 Mon 18:00 Poster E

Influence of defects on hydride formation in thin metal films — •Marc Waninger, Sönke Schmidt, and Astrid Pundt — Instiute of Material Physics, University of Goettingen, Friedrich-Hund-Platz 1, D-37077 Goettingen, Germany

Some metals are capable of absorbing hydrogen in the interstitial sites of the lattice. Additionally, microstructural defects (vacancies, grain boundaries, dislocations etc.) offer sites for hydrogen with binding energies, different from that of the interstitial sites[1].On the one hand hydrogen preferentially dissolves at these defects and they act as hydrogen traps. On the other hand, the incorporation of hydrogen in defects changes their mobility and reduces their repulsive interaction. For dislocations this is known as HELP mechanism, which is important for the hydrogen embrittlement.

In this study, indentation and argon ion bombardment are used to artificially create defects in thin metal films. Indentation is done by using the tip of an atomic force microscope (AFM) and results in dislocation rich volumes underneath the indent. Ar-ion bombardment results in a high density of interstitials and vacancies. These defect rich films are loaded with hydrogen from the gas phase. It is investigated by in-situ AFM, resistivity measurements and x-ray diffraction, if and how the defects affect the hydrogenation behavior of the films.

This research is kindly supported by SFB602, B12 and DFG PU131/9.

[1] A. Pundt, R. Kirchheim, Annual Review Materials Research*36* (2006) 555 - 608.

MM 15.45 Mon 18:00 Poster E

Large Scale Atomistic Simulations on Nanostructure Evolution — •Jeffrey Kelling[1,2] and Karl-Heinz Heinig[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, TU-Chemnitz, Chemnitz, Germany

The Kinetic Metropolis Lattice Monte-Carlo (KMC) method is a means of performing atomistic simulations of self-organization processes in solids at by far larger scales than those accessible via Molecular Dynamics (MD). GPUs currently provide the highest peak processing performance regarding both cost and energy consumption. We present a GPU implementation of KMC achieving up to two order of magnitude higher performance than a sequential reference implementation on a single core of a modern CPU. This enables atomistic simulations at experimental spatiotemporal scales.

MM 15.46 Mon 18:00 Poster E

Simulation of the elastic properties of nanomechanical resonators — •Kristian Scholz, Daniel Mutter, Markus Ring, Ralf Schmid, Martin Vögele, and Peter Nielaba — Physics Department, University of Konstanz, Germany

The oscillation behaviour of Silicon nanomechanical resonators in the form of doubly clamped beams is investigated by Molecular Dynamics simulations using the Stillinger-Weber interaction potential. After setting up the initial structure using a diamond lattice and a (2x1) symmetric dimer surface reconstruction, the end points of the beams are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the beams. Besides varying the size of the beams, the effects of temperature, external stretching fields and cavities are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with length and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the beams into thermal energy of the degrees of freedom of the constituting atoms. Other materials (e.g. NiTi memory alloys) and membranes are explored as well. In order to explore quantum effects in the low temperature regime Path Integral Monte Carlo simulations are performed.

MM 15.47 Mon 18:00 Poster E

Advanced electronic structure calculations of transparent conducting oxide materials — Hemant Dixit, Rolando Saniz, Dirk Lamoen, and •Bart Partoens — CMT and EMAT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

Transparent conducting oxides (TCO) constitute a unique class of materials which combine two physical properties together - high optical transparency and high electrical conductivity. TCOs are widely used in commercial applications such as liquid crystal displays, touch-screen devices, solar cells etc. Thus it is imperative to search for high performance novel TCO materials system. An accurate description of electronic band structure lies at the heart of advanced materials design. Despite of the success demonstrated by ab-initio density functional theory in describing ground state material properties, the key physical property of TCO i.e. the band gap, is poorly described with the standard local density approximation or generalized gradient approximation. Here we will discuss the electronic band structure of prototype TCO materials using advanced electronic structure methods, namely, the state of the art GW approximation and Tran-Blaha modified Becke-Johnson potential scheme. The results obtained for the key physical properties namely the band gap and electron effective mass are discussed along with the position of the 'd' orbitals in the electronic band structure. Such a systematic comparison provides useful insights into the electronic band structure of complex oxide systems and also suggests a recipe for high-throughput materials design.

MM 15.48 Mon 18:00 Poster E

Atom Probe Tomography of Polyelectrolytes and Metall Compounds — •Martin Lütkemeyer — Institut für Materialphysik, Münster, Germany

Laser Assisted Atom Probe Tomography (LA-TAP) with femtosecond lasers has the potential to give chemical and structural information of organic materials like polymers at an atomic scale. We are able to measure and identify poly(acrylic acid) and poly(allylamine hydrochloride) which are deposited on the apex of tungsten tips. The deposition is done by the Layer by Layer technique, in which the tungsten tips are consecutively dipped into poly-anion and poly-cation solutions so that a polyelectrolyte multilayer (PEM) system is build. This procedure enables us to investigate metallic nanoparticles in a new way with the LA-TAP by simply embedding them into the PEM's by dipping the polymer coated tungsten tips into a solution of colloidal nanoparticles. However, due to complex mass spectra and difficult evaporation behaviors of both PEM-matrix and nanoparticles the measurement and reconstruction of these tips is challenging. To demonstrate that it is indeed possible to get chemical and structural information of those materials at such a small scale with the LA-TAP, reconstructions of Au-nanoparticles embedded in PEM's, and corresponding composition profiles and mass spectra will be presented.

MM 15.49 Mon 18:00 Poster E

Origin of the p-type and n-type conductivity in novel spinel transparent conducting oxides ZnX_2O_4 — Mozhgan Amini, Hemant Dixit, Rolando Saniz, Dirk Lamoen, and •Bart Partoens — CMT and EMAT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

ZnM_2O_4 (M=Co, Rh, Ir) spinels are one of the promising p-type transparent conducting oxide (TCO) systems, while $ZnAl_2O_4$ (Gahnite) is considered as a possible n-type TCO. We report the formation energy of acceptor-like (in ZnM_2O_4) and donor-like (in $ZnAl_2O_4$) defects using first principles calculations with an advanced hybrid exchange-correlation functional (HSE06) within the density functional theory (DFT). For ZnM_2O_4 spinels we present results for the cation vacancy and the antisite defect, which are the leading sources of disorder in the spinel structures. We also discuss the band alignments in these spinels.

Further, we have investigated the formation energies of intrinsic defects in $ZnAl_2O_4$ which include the Zn, Al and O vacancy, and the antisite defects: Zn at Al site (Zn_{Al}) and Al at Zn site (Al_{Zn}). The antisite defect Al_{Zn} has the lowest formation energy and acts as a shallow donor, indicating possible n-type conductivity in $ZnAl_2O_4$ spinel by Al doping.

MM 15.50 Mon 18:00 Poster E

Large-area structuring of nanorod arrays by laser interference lithography — •Eric Jehnes[1], Vera Hoffmann[1], René Kullock[2], Gunther Scheunert[3], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Germany — [3]Department of Physics and Astronomy, Queen's University, Belfast, UK

Metal nanorod arrays grown in anodic aluminum oxide show distinct plasmonic resonances, which can be tuned via the rod length, diameter and spacing of the rods [1,2]. However, the influence of structuring (e.g. parallel lines of rods) on the plasmonic properties has not yet been investigated. The work we present concerns the preparation of such structured arrays. To arrange the rods, laser interference lithography is used. This method is able to deliver high-quality periodic photoresist patterns with low defect densities over an area of several cm^2. To integrate the structuring process into the nanorod fabrication, lithography is combined with wet etching and physical vapor deposition. The resulting structures are expected to show new optical properties that can be used to increase the tunability of the plasmonic resonances. Hence, structured arrays find applications in optical waveguides and sensors both for the visible and near infrared range. Furthermore, our technique provides the basis for the low-cost integration of optoelectronic and storage devices based on such nanorod arrays.

[1] R. Kullock et al., Optics Express 16, 21671 (2008) [2] R. Kullock et al., J. Opt. Soc. Am. B 27, 1819 (2010)

MM 15.51 Mon 18:00 Poster E

Molecular Dynamics Simulations on the Coherency of Cu Nano Precipitates in BCC Fe — •David Molnar[1,2], Fabian Maier[1], Peter Binkele[1], and Siegfried Schmauder[1,2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), University of Stuttgart — [2]Stuttgart Research Center of Simulation Technology (SRC SimTech), SimTech Cluster of Excellence, University of Stuttgart

The mechanical behaviour of steels is strongly related to their underlying atomistic structures which evolve during processing or thermal treatment and during their life cycles. In copper-alloyed α-iron, precipitates form within the iron matrix, especially when operated at higher temperatures of above 300°C, yielding a change of the material's mechanical properties. During growth, the approximately spherical precipitates perform a structural transition from bcc to fcc, thus increasing the incoherency between bcc matrix and precipitate. The detailed analysis of this transition on the atomistic length scale by means of Molecular Dynamics simulations is crucial with respect to sequential multiscale coupling with Phase Field Methods and Dislocation Dynamics which are able to simulate particle growth, particle coarsening and the interaction of dislocations with large obstacle fields, respectively. Structural transitions are found to nucleate in the precipitate's centre while the surface is still forced to remain bcc. We will investigate the structural transition of Cu precipitates and the effect on residual stresses and obstacle strength.

MM 15.52 Mon 18:00 Poster E

Full-Scale Modeling of APT Measurement Data — •Christian Oberdorfer, Sebastian Manuel Eich, and Guido Schmitz — Institut für Materialphysik, Münster, Deutschland

The application of simulation enables a complementary approach to the interpretation of measurement results in atom probe tomography (APT). A very first approach to APT simulation was introduced by Vurpillot et al. The approach makes use of an iterative solution of the Laplace equation on a regular grid. Atoms of a modelled field emitter structure are consecutively detached from the surface and respective ion-trajectories are calculated. Consistent with the experimental condition in which a position sensitive detector is placed in front of the emitter sample, the simulated data result in the lateral hit positions of the ions on a simulated detector plane.

The present contribution depicts recent results which were obtained from an extended simulation approach for APT. Founded on an elaborated grid of irregular shaped Wigner-Seitz cells, the potential distribution can be solved without any constraints on the possible emitter geometry. Conceivable emitter structures consist of distinguished lattice types and orientations which reflect realistic atomic distributions. Even the analysis of amorphous structures is possible. Additionally, an adaptive grid of support points allows to extend the simulation space decisively. Ion trajectories with flightlengths of about 10 cm are enabled. — The respective "TAPSim" simulation package is freely offered.

MM 15.53 Mon 18:00 Poster E

Atomistic simulation of a severe plastic deformation-

induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinski[1], Anantha Padmanabhan[2], Martin Peterlechner[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — [2]University of Hyderabad, India

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation or steady-state superplastic flow indicates several unexpected similarities especially with respect to the interface response on the deformation, such as grain boundary (GB) sliding events, which lead to a suppression of dislocation activity. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle GBs in SPD-processed materials in terms of the concept of shear localization in the interfaces and choosing oblate spheroids of a few atomic diameters size as the basic units of sliding. Atomistic simulations of these special GBs are performed. In this approach, the GB is generated, oblate spheroids are defined, extra free volume is introduced, and the oblate spheroids are sheared by a given amount. After this preparation, the whole simulation box is sheared. The GB energy as a function of the extra free volume is determined and the arrangement of the (extra) free volume in the grain boundary is analyzed. The simulation data are compared with experimentally available HRTEM images via calculation of HRTEM images corresponding to simulated GBs and subsequent geometric phase analysis of the local strain fields.

MM 15.54 Mon 18:00 Poster E

Precipitate redissolution in Al-Cu-Li- alloy AA 2195 — •Judith Leese[1], Kathrin Kolotzek[1], Melanie Markgraf[2], and Ferdinand Haider[1] — [1]Universität Augsburg, 86159 Augsburg — [2]Premium Aerotec GmbH

A decrease in density of about 3 wt% for every wt% of Lithium combined with an increase in Youngs modulus of 6 % [1] made the straight path to many applications in aeronautics for Al-Cu-Li alloys. The alloy AA 2195 keeps its superior mechanical properties even at cryogenic temperatures [2]. The strength of this age hardenable Al-Cu-Li alloys is mainly controlled by volume fraction and size of the hardening precipitates like Θ', δ' and T1. Different processes during processing in industry can influence the microstructure of the peak-aged alloy via an short term heat input. The decrease in strength can be assigned to growth and dissolution reactions of the strengthing precipitates. The current study aims to resolve the microstructural processes during heat input for the commercial aluminum alloy AA 2195 at three different temperatures (250°C, 350°C and 510°C). The heating periods were varied from a few seconds to two hours. Vickers hardness measurements characterize the strength of the alloy. DSC measurements allows to monitor further kinetic reactions and TEM was used to record the correspondent changes in microstructure like size and distribution of the relevant precipitates. The combination of the different techniques prooves several reactions like dissolution and Ostwald Ripening during heating. [1] Material Science and Engineering,1980,44(2),213 [2] Journal of Materials Engineering and Performance,1998,7(5),682

MM 15.55 Mon 18:00 Poster E

Ultra thin LiPON layers as an electrolyte for solid-state thin film batteries — •Susann Nowak, Frank Berkemeier, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Despite LiPON (lithium phosphorus oxynitride, $Li_3N_x(PO_4)_{1-x}$) is widely discussed as a suitable electrolyte for all solid-state thin film batteries, there are only a few publications reporting on films that exhibit a thickness below 1 μm. Therefore, in this work we investigate the properties of LiPON films with a thickness between 50 and 500 nm prepared by reactive ion-beam sputtering of Li_3PO_4, using argon as sputter gas and nitrogen as reactive additive and the characterization of the films by temperature-dependent electrochemical impedance spectroscopy (EIS) and transmission electron microscopy (TEM). Temperature dependent measurements of dc-conductivity by EIS give a conductivity of $5 * 10^{-7}$ S/cm at 30° and an activation enthalpy of (58 ± 2) kJ/mol, and hence allow to operate the LIPON films in all-solid state batteries at room temperature, with a reasonable charge/discharge performance. Additionally, thin film batteries have been prepared by depositing a LIPON layer between two metallic electrodes (e.g. Pt and Ag), which are forming a complete electrochemical thin-film cell during the first cycle of cyclic voltammetry measurements.

MM 15.56 Mon 18:00 Poster E

Ion diffusion in lithium titanate thin films — •Fabian Wunde, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Münster

Lithium titanate (LTO) is used as an anode material in lithium ion batteries, as it reveals both, a high ionic conductivity and the capability to reversibly intercalate/deintercalate lithium ions. In our work we use rf-ion beam sputtering to prepare LTO thin films. X-ray diffraction and transmission electron microscopy show, that the layers are crystalline and exhibit a strong orientation in (111) direction, a dense structure, and smooth interfaces. These properties open the possibility to integrate the LTO thin films in all-solid-state lithium ion batteries. On the other hand, the films can be used to study fundamental material properties like lithium ion hopping rates or diffusion coefficients, which are difficult to obtain in case of powder material. In this scope, galvanostatic intermittent titration technique (GITT) is used to determine the chemical diffusion coefficient of lithium within the LTO films. Due to the thin film geometry of the samples, it is possible to reliably evaluate the GITT results via the thin film approach and to determine the lithium diffusivity as function of the lithium concentration.

MM 15.57 Mon 18:00 Poster E

Resonant Photoemission at the O1s threshold to characterize In_2O_3 single crystals — •Jörg Haeberle[1], Matthias Richter[1], Dieter Schmeisser[1], Zbigniew Galazka[2], and Christoph Janowitz[3] — [1]BTU Cottbus, Applied Physics, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Leibniz-Insitut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin Germany

We report on spectroscopic investigations on In_2O_3 single crystals. We focus on the detailed analysis of the O1s resonance profile by resonant photoelectron spectroscopy (resPES). From these we analyze the electronic structure and assign the O2p- and In5sp-state to build the valence band and the conduction band in different contributions, respectively. This is deduced from constant final statespectra on the O-KLL-Auger along the O K-edge and In $M_{4,5}$-edge and a comparison to the corresponding X-ray absorption spectroscopy data. We also identify several types of defects. A broad band of oxygen derived defects is identified in the valence band and extends throughout the gap. Small polarons are attributed to cause an anti-resonance in the constant initial states around the O1s threshold. In addition, an Auger decay separated by the O-KLL is present at O-K resonance and indicates the existence of localized charge transfer states which involves In5sp states. Finally, we are able to distinguish two different oxygen species from the resPES data. One corresponds to theintrinsic In_2O_3 structure and the other is a non-corresponding species.

MM 15.58 Mon 18:00 Poster E

Characterisation of residual stress in steel components with non-destructive evaluation methods — •Sascha Raatz[1], Farid Hendry[1], Angga Ginandjar[1], Michael Kaack[2], Peter Staron[3], Michael Hofmann[4], and Katharina Theis-Bröhl[1] — [1]University of Applied Sciences Bremerhaven, 27568 Bremerhaven — [2]Salzgitter Mannesmann Forschung GmbH, 47259 Duisburg — [3]Helmholtz-Zentrum Geesthacht, 21502 Geesthacht — [4]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, 85747 Garching

In industrial application non-destructive evaluation methods are widely used to determine residual stress to prevent failure under load. Magnetic Barkhausen noise (MBN), harmonic analysis and ultrasonic are favoured due to their simple onsite applicability with portable devices. But all those techniques have different limitations and require an independent calibration by an absolute evaluation method like X-ray- and neutron-diffraction. In our study we compare all those techniques to determine the residual stress in steel components. The chosen samples are low-alloy steel pipes with different levels of a straightening process which leaves a visible helix on the surface. This helix is measurable with MBN and harmonic analysis which are sensitive on the skin of the surface. We used synchrotron- and neutron-diffraction to get absolute values in the bulk of our samples. The residual stress correlates with the MBN results, the levels of straightening and changes its value up to 400 MPa through the wall-thickness. We acknowledge funding by BMBF, DESY, FRM II and HZG. The samples were provided by our industrial partner SZMF.

MM 15.59 Mon 18:00 Poster E

Elastic-to-plastic transition: waiting time analysis of long term creep measurements — Jon-Olaf Krisponeit[1], Karina

E. Avila[2], •Sebastian Pitikaris[1], Stefan Küchemann[1], Antje Krüger[1], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Department of Physics and Astronomy, Ohio University, Athens, OH, 45701, USA

We studied the elastic-to-plastic transition of the bulk metallic glass $Pd_{77.5}Cu_6Si_{16.5}$ under uniaxially applied tensile stress. The crossover from initially elastic behavior via small plastic events to cooperative processes resulting in the emergence of macroscopic shear bands and even catastrophic failure is a very interesting phenomenon from both a materials science viewpoint and in fundamental physics. In theory, the statistic properties of avalanche-like slip events are studied intensively.

We recorded long term creep measurements (up to one week) under constant stress. Although single slip events–like activations of a shear transformation zone–are undetectable in macroscopic experiments, their cooperative avalanche-like motion is reflected in waiting time statistics. A numerical waiting time analysis was implemented and power-law behavior was found in the frequency distribution of waiting times. In addition, also power spectra have been analyzed. The results are discussed in terms of a transition from uncorrelated slip avalanches to the formation of shear bands.

We acknowledge financial support for this work by DFG via SFB 602 and FOR 1394.

MM 15.60 Mon 18:00 Poster E

Phase field modeling of interdiffusion microstructures in Ni-base superalloys — •Leslie Mushongera, Micheal Fleck, and Heike Emmerich — University of Bayreuth

The effect of the refractory element rhenium(Re) on the kinetics of coarsening in negatively misfitting ni-based superalloys during heat treatment is studied. A multicomponent phasefield model coupled with inputs from thermodynamic and kinetic databases to provide the relevant driving forces is developed. In order to realistically capture the complex nature of interdiffusion, the CMSX4 and CMSX6 superalloys with well-defined weight percent contents are analyzed.

Microstructural evolution is first studied in the presence of a lattice misfit with inhomogeneous elastic constants. Cuboidal precipitates arranged in a square array are formed. We then study the system under external load along a cubic axis. It is observed that the precipitates become anisotropic and the orientation differs depending on the sign of the applied stress. Simultaneously, we determine the mechanism by which Re reduces coarsening. It is seen that Re additions substantially reduce the rate of precipitate coarsening by keeping their shape almost cuboidal, which is the interfacial energy minimizing configuration. Re also reduces coarsening by hindering the growth of the rafts. In addition,we derive stereological measures to characterize the kinetics of coarsening.

MM 15.61 Mon 18:00 Poster E

KKRnano: Improvements in efficiency and order-N scaling for use on massively parallel computers — •Elias Rabel, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Petascale high-performance computers open completely new opportunities for the first-principles treatment of materials problems. The recently developed code KKR*nano* [1] implements the screened KKR Green's function method for DFT calculations of unit cells with thousands of atoms. It targets modern supercomputing architectures, which requires being able to utilise more than 100000 processors.

The KKR method considers multiple scattering of partial waves up to a maximum angular momentum $\ell_{\max}$. We investigate the structure of matrices with sparse block structure occuring in the treatment of very large unit cells. A distance dependent angular momentum cutoff is employed to reduce the effective matrix size with little compromise in accuracy. The special case of neglecting all partial waves at reasonably large distances leads to an $O(N)$-scaling method.

Usage of an iterative solver necessitates an appropriate preconditioning strategy. A block-circulant preconditioner has been proven to be highly effective in the case of uniform block sizes. Solution strategies for the case of the distance dependent ℓ-cutoff, where one has to deal with variable block sizes, are currently under investigation.

[1] A. Thiess *et al.*, Phys. Rev. B **85**, 235103 (2012)

MM 15.62 Mon 18:00 Poster E

Investigation of ionic surfactants capability in dispersion of multi-walled carbon nanotubes in an aqueous solution — •Maryam Khazaee[1,2], Anindya Majumder[3], Larysa Baraban[1], Joerg Opitz[1,3], and Gianaurelio Cuniberti[4] — [1]Institute for materials science and max bergmann center of biomaterials, TU dresden, 01062 dresden, germany — [2]Leibniz institute for crystal growth,12489 berlin, germany — [3]Fraunhofer institute IZFP dresden, 01109 dresden, germany — [4]Division of IT convergence engineering, POSTECH, pohang, korea

We present a comparative investigation of a dispersion of multi-walled carbon nanotubes (MWCNTs) in various ionic surfactants including three anionic and two cationic ones. The optimum sonication conditions for the dispersion of MWCNTs have been determined. Among these surfactants- Sodium dodecyl sulfate (SDS), Sodium dodecylbenzenesulfonate (SDDBS), Sodium cholate (SC), Dodecyltrimethylammonium bromide (DTAB) and Decyltrimethylammonium bromide (CTAB)- SDDBS and DTAB provided maximum and minimum dispersion susceptibility, respectively, which has a good agreement with their chemical structure properties. Dispersion efficiency of CNTs was quantified via determining extinction coefficients of these MWCNTs, derived from UV-Vis spectra. The dispersion efficiency of MWCNTs was characterized by transmission electron microscopy (TEM), UV-Vis spectroscopy and atomic force microscopy. These results serve as future guide for utilization of MWCNTs in their different applications such as nanocomposits, nanoelectronics, biosensor, etc.

MM 15.63 Mon 18:00 Poster E

Crystal growth and characterization of $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ — •Stephan Pohl, Céline Grimm-Allio, Carola Dietrich, Klaus-Dieter Luther, Franz Ritter, Wolf Assmus, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

The clathrate $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ possesses interesting thermoelectric properties [1]. On the one hand it features a high electric conductivity, on the other hand it has a low thermal conductivity. These properties are due to the specific crystal structure with Ba guest atoms in a Ni-Ge host lattice and might be promising towards technical applications. Neutron scattering techniques are well suited to investigate the phonon dispersions to unravel the underlying microscopic origin of the thermoelectric characteristics. However, large single crystals are required for that kind of research. Here, we show that the crystal growth of $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ can be achieved by the crucible-free Czochralski pulling method. We particularly present the crystal growing achievements with a tungsten single crystal as a seed and the results of x-ray investigations on the obtained single crystals.

[1] L. T. K. Nguyen *et al.*, Dalton Trans. **39**, 1071 (2010).

MM 15.64 Mon 18:00 Poster E

Optimization of Fe/MgO/Fe Interfaces by Atom Probe Tomography — •Rabab Bahabry, Torben Boll, Ryota Gemma, and Talaat Al-Kassab — King Abdullah University of Science & Technology, Division of Physical Sciences and Engineering, Thuwal, 23955-6900, Kingdom of Saudi Arabia

As part of an emerging nanotechnology, devices based on the Tunnel Magneto-Resistance (TMR) effect have promising applications. The metal/oxide interfaces govern the magnetic properties of such multilayer structures. Hence, Atom Probe Tomography (APT) and STEM investigations help clarifying any chemical or structural inhomogeneity of these layer structures. In this paper Fe/MgO/Fe layer structures were deposited on Si-microtip coupons and W-tips by various ion beam sputtering techniques. Results obtained on several samples with differing deposition conditions utilizing the local electrode atom probe LEAP 4000 HR, which was installed recently at the King Abdullah University of Science & Technology. Results are presented and discussed in view of the influence of deposition conditions on the quality of prepared multilayer stacks.

MM 15.65 Mon 18:00 Poster E

Ab-initio prediction of the critical thickness of a coherent precipitate — Sankari Sampath, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-University Bochum

Segregation and precipitation of second phases in metals and metallic alloys are complex phenomena with a high influence on the mechanical properties of the material. Models exist that describe the growth of coherent, semi- and incoherent precipitates. One of the parameters of these models, namely the energy of the interface between matrix and precipitate is investigated in more detail in this project.

Our example is a metastable Mo-C phase, the body-centered tetrag-

onal structure, which has been observed experimentally by high-resolution electron microscopy as a semi-coherent precipitate [1]. It is assumed that it is stabilized by the precipitate interface energy. Furthermore, this interface is supposed to change from coherent to semi-coherent during the growth of the precipitate. We predict the critical thickness of the precipitate by calculating the different contributions to a semi-coherent interface energy by means of ab-initio density functional theory calculations. The parameters in our model include the elastic strain energy stored in the precipitate as well as a misfit-dislocation energy that depends on the dislocation core width and the dislocation spacing. Our predicted critical thickness agrees well with experimental observations.

[1] J.M. Pénisson, M.Bacia, M.Biscondi, Phil. Mag. A 73, 859 (1996).

MM 15.66 Mon 18:00 Poster E

Influence of Quenching & Partitioning on the Volume Fraction of Austenite Phase in Steel using X-ray Diffraction — •Karin Rüster[1], Andre Steffen[1], Michael Paulus[1], Christian Sternemann[1], Metin Tolan[1], Niko Grosse-Heilmann[2], Christian Kronholz[2], and Andreas Peters[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Benteler Tube Management GmbH, 33104 Paderborn, Germany

Steel is a common material in our daily life. Macroscopic characteristics (e.g. hardness, tensile properties) of steel are affected by the crystalline structure, i.e. austenite and martensite phase, which is changed during heat treatment. During the process of Quenching and Partitioning carbon diffuses from martensite to austenite and thereby stabilises the phase of austenite. This way a microstructure with retained austenite is produced. To investigate the material's characteristics XRD-experiments have been carried out at beamline BL9 of the synchrotron light source Delta, in Dortmund. A gain of retained austenite with increasing holding time is observed ex situ in pre-treated samples. Changes of the volume fraction of austenite during the process of heating and cooling were analyzed in situ. The stabilisation of austenite and an increase of the lattice constant both induced by the carbon diffusion was observed.

MM 15.67 Mon 18:00 Poster E

An apparatus for the synthesis of cluster-based materials — •Arne Fischer, Herbert Gleiter, and Horst Hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany

A new cluster deposition system for the synthesis of materials composed of mass-selected clusters embedded in matrices of other materials as well as cluster-decorated surfaces was constructed and first deposition experiments were performed.

The system covers a large range of cluster sizes from single atoms up to clusters consisting of several thousands of atoms and the resulting cluster beam has a narrow size distribution. During the deposition the number of clusters as well as their impact energy is well defined. Hence this approach can open pathways to a new class of materials with tailored electronic, magnetic or catalytic properties.

As a first experiment iron clusters were deposited into a silver matrix. The immiscible system Iron-Silver is a well-known GMR material. In contrast to the production via e.g. MBE where only the composition is defined with our approach we have on top control over the size of the embedded clusters. Hence it allows studying the GMR effect as a function of cluster size and density in the material. Various samples with cluster sizes from 500 to 2000 atoms and different concentrations of clusters were produced and characterized with a SQUID magnetometer. The first results look promising and prove the exceptional capabilities of our new cluster deposition system.

MM 15.68 Mon 18:00 Poster E

In detail 3D Atom Probe investigation of Tantalum capped CoFeB layers — •Patrick Stender, Houari Bouchikhaoui, and Guido Schmitz — Institut of Materials Physics, WWU, Münster, Germany

The tunnel magnetoresistance (TMR) is an important physical effect used in current technology. The TMR ratio is influenced by various parameters. Very high TMR ratios can be obtained in CoFeB/MgO based magnetic tunnel junctions. However, the TMR is strongly influenced by the capping material. Choosing Tantalum as a capping material, the TMR can be increased drastically, after a defined heat treatment. We present an atom probe study of a model MgO/ CoFeB/Ta system. In the as-prepared state, the CoFeB layer exhibits an amorphous structure Different Isochronal and isothermal annealing sequences have been carried out to investigate the structural changes and reactions. Observed diffusion and segregation processes of Boron have been identified and quantified.

MM 15.69 Mon 18:00 Poster E

A molecular dynamics study of crack/void interaction in α-Iron — •Tianxiang Liu, Sebastien Groh, and Abdolhamid Attaran — Institute for Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Lampadiusstr. 4, 09596 Freiberg, Germany

When a crack front interacts with an array of a second-phase inclusions, it bends to an angle before it moves furthers. Depending on the strength of the inclusions, the crack front either remains relatively straight or bows between inclusions and moves deeply along the easy path. The resistance to crack growth is therefore changed by the presence of inclusions.

In this paper, we are presenting a study on crack/void interaction using molecular dynamics. α-iron modeled with an EAM potential was considered. Three distributions of void were considered: (i) void positioned at varying distance normal to the crack tip, (ii) void inserted at varying distances along the crack-tip and (iii) void placed in such a way that dislocations nucleated at the crack tip reached the void when moving. The data obtained for the different configurations were compared to the ones obtained in a void free specimen.

Depending on the configuration, elastic shielding or anti-shielding was observed as a function of the temperature and strain rate. The increase in temperature would augment the shielding effect in all the configurations. The anti-shielding effect was detected in the first configuration. This effect diminished as the void was moved away from the crack tip as expected by elasticity.

MM 15.70 Mon 18:00 Poster E

$SrRuO_3/Pr_{0.7}Ca_{0.3}MnO_3$ epitaxial multilayers: A HAADF-STEM, EDX and image simulation study — •Eckhard Pippel[1], Reinald Hillebrand[1], Ionela Vrejoiu[2], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle (Saale), Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

The electrical and magnetic properties of perovskite multilayer structures strongly depend on the interface morphology between the single layers. We study the interfaces of PLD-grown epitaxial multilayer stacks of $SrRuO_3/Pr_{0.7}Ca_{0.3}MnO_3$ (SRO/PCMO) by means of probe-corrected (C_s=0) scanning transmission electron microscopy (HAADF-STEM) including energy dispersive X-ray analysis (EDX). It is possible to clearly distinguish different chemical terminations of the single layers as well as varying degrees of intermixing, if image simulations are utilized. The interfaces are evaluated by matching the intensities of the related atomic columns with simulated HAADF-STEM patterns of crystallographic super-cell models, supported by atomically resolved chemical analysis (EDX). All these techniques proved the interfaces to be affected by intermixing over two (PrO-terminated) or one (SrO-terminated) lattice planes. In practice, a series of annealing experiments of the SRO/PCMO specimens was performend to find out the temperature stability of these perovskite multilayers. The temperatures applied were between 725°C and 1200°C. In summary it is stated that already Z-dependent HAADF-STEM images offer a fairly good atomically resolved insight into intermixing phenomena.

MM 15.71 Mon 18:00 Poster E

Mechanical influences on lithium ion battery electrodes — •Tobias Kitzler[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholz-Zentrum Geesthacht, Institut für Werkstoffmechanik, Werkstoffforschung — [2]TU Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

Lithium ion batteries have drawn major attention during the last years. One very promising attempt to get batteries with better performance is to reduce the structure size of the electrodes which leads to very high surfaces and therefore improved kinetics. Besides this, downscaling seems to be a promising way to omit crack formation due to volume change which is the most important capacity loss mechanism in lithium alloy negative electrodes. On the other hand, downscaling leads to mayor stress evolution due to volume change, which according to the thermodynamic Maxwell relations, changes the electrochemical potentials. This influence has been observed in different experiments, but was not yet quantitatively measured. Here a setup is presented which allows to quantitatively measure the influence of uniaxial strain

on the electrochemical properties of lithium ion electrodes. Therefore, dense and nanoporous Au films, synthesised by sputtering of pure Au and Au32Ag68, followed by an electrochemical dealloying process respectively, on a polyimide substrate were oscillatory strained and the corresponding change of the chemical potential recorded and analysed with respect to its impact on the kinetics of the loading and unloading processes as well as microstructural changes of the electrode itself.

MM 15.72 Mon 18:00 Poster E

Transmission electron microscopy study of defects in BiFeO3 thin films — •Hakan Deniz, Akash Bhatnagar, Eckhard Pippel, Marin Alexe, and Dietrich Hesse — Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany

A wide class of oxide materials with perovskite crystal structure has been in the focus of intense research efforts lately due to fascinating properties they posses; such as ferroelectricity, colossal magnetoresistance, superconductivity, etc. Bismuth ferrite (BiFeO3) among them is the leading contender in the research of multiferroic compounds with both ferroic order parameters well above room temperature. It is of vital importance to grow defect-free high quality thin films in order to better understand/correlate structure-property relationships of these materials. Single crystal BiFeO3 thin films grown by pulsed laser deposition on scandate oxide substrates (TbScO3, GdScO3, etc.) have been investigated in high-resolution TEM (HRTEM) and high angle annular dark field scanning TEM (HAADF-STEM). Defects having a layered structure, similar to bismuth-oxide layered perovskites, with a chemical composition different from the rest of the film have been observed. Fast Fourier transform (FFT) analysis and image processing were used to elucidate the nature of these defects. They correspond to a new unknown phase in BiFeO3 thin films. Understanding their origin will help to grow higher quality virtually defectless films. This work is supported by the FP7 project IFOX.

MM 15.73 Mon 18:00 Poster E

In situ transmission electron microscopy study of the crystallization of bits in Ag4In3Sb67Te26 — •Manuel Bornhöfft[1,2], Andreas Kaldenbach[3], Matthias Wuttig[3], and Joachim Mayer[1,2] — [1]Central Facility for Electron Microscopy, RWTH Aachen University, Aachen, Germany — [2]Ernst Ruska-Centre, Forschungszentrum Jülich, Jülich, Germany — [3]I. Physikalisches Institut (IA), RWTH Aachen University, Aachen, Germany

The understanding of crystallization kinetics of phase-change materials is mandatory to develop reliable and fast phase-change data-storage devices, which can surpass actual data-storage technologies. A topic of interest is the role of nucleation and growth in phase-change materials at different conditions.

In this work in situ-methods in a transmission electron microscope are used to observe the crystallization of round amorphous marks (bits) in a crystalline matrix of the phase-change material Ag4In3Sb67Te26. The in situ-methods employed are based on crystallization by in situ-heating and in situ-irradiation by the focused electron beam in the microscope. The bits with 0.6 μm in diameter are produced by laser irradiation of a 30 nm thick crystalline layer of the phase-change material. The phase-change layer is embedded in a 160 nm thick supporting multilayer stack. The supporting layers are amorphous and the phase-change layer is crystallized through ex situ-heating.

The results are compared with experimental observations on Ge2Sb2Te5 and give important insight in the crystallization mechanisms and the underlying thermodynamic processes.

MM 15.74 Mon 18:00 Poster E

TEM study of annealed γ-Al_2O_3-coatings for cutting tools and of γ-Al_2O_3-coated cutting tools after the use in cutting tests — •Merlin G.J. Müller[1], Joachim Mayer[1], Susanne E. Cordes[2], Kirsten Bobzin[3], Nazlim Bagcivan[3], Mara Ewering[3], and Ricardo H. Brugnara[3] — [1]Central Facility for Electron Microscopy, Aachen, Germany — [2]Laboratory for Machine Tools and Production Engineering, Aachen, Germany — [3]Surface Engineering Institute, Aachen, Germany

Among the transition aluminas, the γ-Al_2O_3-phase has a high potential for the use as hard coating in many technological applications, because it exhibits excellent properties e.g. high hot hardness and high thermal stability. It can also be deposited by means of physical vapor deposition at lower temperatures (below 700 °C) than the stable α-Al_2O_3 phase, deposited by means of chemical vapor deposition (about 1000 °C). Thus, even temperature sensitive materials can be coated and the resulting alumina layer is rather fine-grained which should lead to better mechanical properties. The phase transformation of the metastable γ-Al_2O_3-phase into the stable α-Al_2O_3-phase at high temperatures can cause cracks or even the delamination of the coating. To investigate the phase stability of γ-Al_2O_3-coatings, the structure of annealed samples and of samples after the use in cutting tests were characterized by Transmission Electron Microscopic-methods. The γ-Al_2O_3-coatings were deposited by means of Magnetron Sputter Ion Plating on cutting inserts with a (Ti,Al)N-interlayer or directly onto Si-wafers.

MM 15.75 Mon 18:00 Poster E

Ultrathin TEM lamellae for low voltage Cs-corrected STEM — •Andriy Lotnyk, David Poppitz, Ulrich Ross, Jürgen W. Gerlach, Eric Thelander, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Permoserstr. 15, 04318 Leipzig, Germany

For high-resolution aberration-corrected (Cs-corrected) low voltage scanning transmission electron microscopy (STEM) the quality of investigated TEM samples is crucial. The TEM specimens should be thinner as 10 nm. Nowadays, widely used focused ion beam (FIB) preparation techniques cannot be employed in fabrication of thin TEM samples with a thickness less than 10 nm. In the present work, we investigate the preparation of different thin film materials and interface structures for analysis in low voltage Cs-corrected STEM using FIB lift-out method followed by low energy Ar-ion polishing (less than 1 kV) in a NanoMill low energy ion mill system. Using this approach we are able to routinely prepare large area TEM lamellae with thicknesses below 10 nm. The resulting TEM specimens are suitable for low voltage STEM. We have demonstrated atomic resolution by Cs-corrected STEM at 80 kV.

MM 15.76 Mon 18:00 Poster E

Study of Solid Solution Strengthening of Nickel by transition metal solutes using Diffusion couples and Nanoindentation — •Hamad ur Rehman, Mathias Göken, and Karsten Durst — Institute of General Materials Properties, Department of Material Science, FAU erlangen-Nürnberg

Diffusion couples are often used for the determination of phase diagrams. In the present work, nanoindentation was used on diffusion couples to measure solid solution strengthening in Nickel based alloys. By combining Nanoindentation with the chemical composition, measured by EDX a very high spatial resolution is achieved in the Interdiffusion zone. It was applied to the development of Nickel based super alloys, which have more than 15 alloying elements. While some of these are gamma prime formers, others act as solid solution strengtheners for the matrix. Therefore, it is important to understand the contribution of these alloying elements on solid solution strengthening. Ni-NiX (X = Ta, W, Re, Ir and Pt) diffusion couples were used to study the influence of transition metal elements on solid solution hardening (SSH) of Nickel. The SSH was evaluated using Labusch theory. It was found that the solid solution hardening coefficient is dependent on the size of the solute elements and their atomic number. These results show that the solid solution strengthening depends on the atomic radius and the corresponding electronic structure of the solute elements. This combinatory approach allows us to determine the SSH coefficients as a function of the composition of the solid solution hardening element.

MM 15.77 Mon 18:00 Poster E

Characterizing the origin of the collapse of the channeling circle in aberration-corrected HRTEM — •Alexander Surrey[1,2], Darius Pohl[1,2], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany. — [2]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

Calculations of the complex electronic exit wave functions (EWFs) of model structures utilizing multi-sclice algorithms in combination with HRTEM contrast simulations reveal that the amplitudes and phases of these reconstructed EWFs lead to a collapse of the channeling circle when "real" samples are investigated under realistic microscopy conditions. As a consequence, the reconstruction of the 3D structure of the samples by means of the acquisition of focal series of HRTEM images becomes impossible. A detailed analysis shows that this collapse is caused by the accumulation of contributions from (i) the modulation transfer function of the camera, (ii) slight misorientations of the sample, (iii) inelastic absorptions, (iv) amorphous overcoats or substrates, and (v) equilibrium as well as athermal phononic excitations. The collapse becomes most easily evident from a significant lack in the phase signal derived from the EWFs. Whereas the phase shift asso-

ciated with moving along the channeling circle in the Gaussian plane should successively grow to the full range of 2π, the phases determined from the EWFs frequently amount to only fractions of π. This limited phase range is confirmed by the EWF recontructions determined from experimental through focus series of thin Au nanostructures acquired with an aberration-corrected FEI Titan^3 80-300 microscope.

MM 15.78 Mon 18:00 Poster E

Investigation of metal droplets on dilute Bi-containing III-V semiconductors — •Eduard Sterzer, Nikolai Knaub, Peter Ludewig, Wolfgang Stolz, and Kerstin Volz — Material Sciences Center and Department of Physics, Philipps-University Marburg, Germany

Dilute bismuth (Bi)-containing III-V semiconductors are interesting from the application point of view, as Bi increases the spin-orbit splitting in conventional III-V semiconductors. The epitaxial growth of these materials is a big challenge due to the formation of metal droplets on the surface. In order to grow droplet free layers a better understanding of the formation process of these droplets is necessary. In this study the surface morphologies of Ga(BiAs)/GaAs structures grown by metal organic vapor phase epitaxy are investigated by scanning electron microscope and atomic force microscope (AFM). Energy dispersive X-ray spectroscopy was used to determine the composition of the droplets. Furthermore the crystal structure was analysed by transmission electron microscopy (TEM). In dependence on the V/III ratio as well as the growth temperature we observe pure Bi- droplets or mixed Ga-Bi droplets. The investigation of the morphology using AFM gives an indication of the droplets moving on the surface during growth. The crystal structure around the droplets and the structure of the droplets itself was investigated with transmission electron diffraction as well as high resolution TEM and will be correlated to the growth conditions.

MM 15.79 Mon 18:00 Poster E

TEM dark-field characterization of anti phase domain boundaries in GaAs on Ge — •Lukas Nattermann, Tatjana Wegele, and Kerstin Volz — Structure and Technology Research Laboratory, Materials Science Center and Faculty of Physics Philipps-Universität Marburg, Germany

The use of GaAs on Ge in multijunction solar cells requires a high crystal quality and a defect-free GaAs/Ge interface. For the characterization of the GaAs-layer and the GaAs on Ge boundary we used transmission electron microscopy (TEM). Additionally we compared GaAs on Ge to GaP on Si with respect to the anti phase domain (APDs) boundaries. In order to investigate the influence of such growth-parameters as temperature and the atom types in the monolayer between GaAs and Ge, three MOVPE (metal organic vapour phase epitaxy)-grown GaAs/Ge - samples were examined by using the TEM dark-field (DF)-technique. To verify APDs with the help of contrast reversal we used the (002)- and (00-2)-DF-reflections. We study specimens in three different zone axes, [001], [110] and [1-10], to get an idea of the three dimensional shape of the anti phase domains. We can show the difference of the shape of APDs in GaAs on Ge and GaP on Si and the influence of the insufficient pretreatment of the Ge-substrate. Moreover we determine the directions of the propagation planes of the APD-boundaries and analyze the size of the APDs.

MM 15.80 Mon 18:00 Poster E

Quantitative study of electron-radiation damage by in situ EFTEM investigations of the phase transformation from $CaCO_3$ to CaO at 80 kV, 40 kV and 20 kV — •Werner Schweigert[1], Ute Golla-Schindler[1], Gerd Benner[2], and Ute Kaiser[1] — [1]Group of Electron Microscopy of Materials Science, Central Facility of Electron Microscopy, 89081 Ulm, Germany — [2]Carl Zeiss NTS GmbH, Application TEM / Materials Analysis, 73447 Oberkochen Germany

The TEM investigation showed that under electron irradiation a phase transformation from $CaCO_3$ to CaO occur. (This is the transformation route for CaO (quicklime) production out of calcite, taking place at elevated temperatures of 900 °C.) The phase transformation is accompanied by a strong volume loss of the particles. We developed a method for measuring quantitatively the volume loss in dependence of the particle thickness and the accelerating voltage of the microscope. The determination of the volume is divided in two parts. Our method for segmenting the image into vacuum and particle is an edge detection process based on the canny algorithm. The thickness can be measured with the log-ratio method. The TEM investigations were performed on the SALVE (Sub-Angström Low-Voltage Electron) prototype microscope equipped with an image-side Cs-corrector, a field emission gun, a monochromator and a corrected in-column OMEGA energy filter. TEM studies were performed at 20, 40, 80 kV. We found that the volume-loss is dose-rate dependent and increases with lower voltages; the contrast however is increasing.

MM 15.81 Mon 18:00 Poster E

Electron irradiation effects on QDs in TEM and SEM — •Thomas Kister, Ute Golla-Schindler, and Ute Kaiser — Group of Electron Microscopy of Materials Science, Central Facility of Electron Microscopy, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Monodisperse CdSe/CdZnS QDs, which are capped with trioctylphosphine oxide (TOPO), have a high fluorescence quantum yield. They are for example supposed to be used in the near future as marker for biological matter in medicine. Up to now the chemical and structural constitution on the atomic level is not well known. Unfortunately, in the initial investigation it was indicated that QDs are losing their fluorescence abilities dramatically by electron irradiation already at low dose rates. Therefore we started systematic studies of radiation damage dependence on dose, dose rate and accelerating voltage. For the experiments the TOPO-capped QDs, which are suspended in hexane, are deposited on carbon and silicon oxide filmed TEM-grids. The fluorescence of the QDs is measured before and after electron irradiation with an optical microscope (Zeiss Axioscope 2 mot plus). A Philips CM20 TEM and a Zeiss NVision 40 SEM are used for the electron irradiation investigations. Through these experiments we hope to get a better understanding of the interaction and irradiation mechanisms taking place during the electron microscopy studies.

MM 15.82 Mon 18:00 Poster E

Reduction of Radiation Damage in Ultrathin MoS_2 — •Mona Sedighi, Simon Kurasch, Gerardo Algara-Siller, and Ute Kaiser — Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm, Germany

Previous high-resolution transmission electron microscopy (HRTEM) experiments [1] on free-standing single layer MoS_2 reported that, at an acceleration voltage of 80 kV, the material suffers from knock-on damage via removal of sulfur atoms from the beam exit surface. Similar to earlier work on graphene [2] it is possible to extract the sputtering cross section from atomically resolved HRTEM time series.

Here we report that, covering the electron exit surface of the free-standing single-layer MoS_2 by single-layer graphene serves to minimize the radiation damage. Moreover, comparing the response to high electron irradiation of free-standing MoS_2 to top-side covered and bottom-side covered MoS_2 allows separating the effect of ionization and chemical damage from the total damage that initially was attributed only to sputtering.

[1] H. Komsa et al., Phys. Rev. Lett 109, 035503 (2012)
[2] J. Meyer et al., Phys. Rev. Lett 108, 196102 (2012)

MM 15.83 Mon 18:00 Poster E

Voltage contrast in SEM for revealing charge transport through metallic nanowire transparent electrodes — •Stefanie Spallek[1], Johannes Krantz[2], Peter Kubis[2], Johannes Holzmair[3], Silke Christiansen[3], Christoph J. Brabec[2], Benjamin Butz[1], and Erdmann Spiecker[1] — [1]CENEM, University of Erlangen-Nürnberg — [2]I-MEET, University of Erlangen-Nürnberg — [3]MPI for the Science of Light, Erlangen

Metallic nanowire (NW) transparent electrodes are of special interest in research and economy due to their cheap and scalable printing production process, their high optical and electrical quality and their application possibility to flexible devices. However charge transport through metallic NW networks is not yet well understood. Here, we report on a voltage contrast dependent scanning electron microscopy (VC-SEM) study of metallic NW electrodes near the electrical percolation threshold. As the properties of NW junctions within the network directly lead to the properties of the whole electrode, e.g. sheet resistance, they are of special interest in this study. NW junctions are insolating until the voltage threshold is reached, whose value presumably is depending on the insulating layer of process residues. By exceeding the voltage threshold the NW junction seems not to balance the amount of charge carriers on both sides, though. Therefore, the contrast mechanism of VC-SEM of metallic NWs was studied to quantify the voltage difference. In addition we show a VC-SEM study of metallic NW electrodes ready for application with which a potential drop of 0 to 8 Volts over a distance of several microns was observed.

MM 15.84 Mon 18:00 Poster E

Freely suspended membranes from epitaxial graphene on silicon carbide — •Christian Dolle[1], Benjamin Butz[1], Daniel Waldmann[2], Heiko Weber[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg

We present a route to produce freely suspended graphene membranes by thermal decomposition of SiC(0001) at 1760° C under reduced inert gas atmosphere yielding a mean of 1.2-1.5 layers of high crystalline-quality graphene. Laser-assisted electro-chemical removal of the SiC substrate in KOH at lithographically predefined areas allows us to tailor the number and shapes of the membranes with sizes up to at least 500 μm^2. We carried out a thorough characterization of the freely-suspended membranes employing Raman spectroscopy, SEM, low-kV-STEM and plan-view TEM. The powerful tool of abberation-corrected TEM can resolve the spatial distribution of one up to four graphene layers on the membranes and contrast variation in dark-field imaging allows a straightforward and facile assignment of the number of layers. One of the great benefits of the preparation procedure is the high cleanliness of the samples, allowing high resolution imaging even without the need of precedent heat treatment although the membranes withstand in-situ thermal exposure up to 1000° C in vacuo without mentionable damage.

MM 15.85 Mon 18:00 Poster E

Structural Analysis of Nickel Doped Cobalt Ferrite Nano Particles Prepared by Coprecipitation Method — Mahbube Houshyar[1], •Ali Alidoust[1], Zohre Askari[1], Zahra Jafari[1], and Fateme Zebhi[2] — [1]Shahid beheshti,Tehran,Iran — [2]Semnan,Semnan,Iran

in this research nano particles of cobalt ferrite ,nickel cobalt ferrite and nickel ferrite have been synthesized using coprecipitation method. size of the every particles have been obtained by XRD and analyses of UV , FTIR , SEM , DLS and VSM have been done on the nano powders and the size , light absorption , dynamic light scattering , coercivity , retentivity and saturation magnetization of the particles have been compared.

MM 15.86 Mon 18:00 Poster E

In-situ and ex-situ ACOM-STEM analysis of the direction dependent deformation behavior of nanotwinned copper — •Aaron Kobler[1,2], M. Funk[3], C. Eberl[3], A. Hodge[4], Horst Hahn[1,2], and Christian Kübel[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, 76021 Karlsruhe, Germany — [2]Technische Universität Darmstadt (TUD), KIT-TUD Joint Research Laboratory Nanomaterials, 64287 Darmstadt, Germany — [3]Karlsruhe Institute of Technology (KIT), Institute of Applied Materials, 76021 Karlsruhe, Germany — [4]University of Southern California, Department of Aerospace and Mechanical Engineering, Los Angeles, California 90089-1453, USA

Nanotwinned (nt) metals as a class of nanostructured materials have been receiving considerable attention as they combine the high strength of nanocrystalline (nc) metals with a higher ductility and higher thermal stability compared to the corresponding nc metals. Face-centered cubic metals with low stacking fault energy like Cu have the tendency to develop this kind of nt structure. Although twin boundaries are thermodynamically more stable than random grain boundaries, they can become unstable under mechanical load. The deformation behavior of magnetron sputtered nt Cu was studied using ex-situ and in-situ TEM techniques combining classical BF/DF-TEM analysis with the recently developed automated crystal orientation mapping (ACOM-TEM). Two straining directions were tested in-situ, one parallel to the twin plane and one perpendicular to it and compared to the ex-situ deformation parallel to the twin plane on ~20μm thick bulk samples. The straining experiments show a significant difference between bulk and thin film deformation as well as a strong orientation dependence in the thin film.

MM 16: Invited Talk (Hauptvortrag): Takeuchi

Time: Tuesday 9:30–10:00 Location: H24

Invited Talk MM 16.1 Tue 9:30 H24

Combinatorial approach to multifunctional materials — •Ichiro Takeuchi — University of Maryland, College Park, MD, USA

We have developed a thin-film based high-throughput methodology for rapid screening of large compositional phase spaces in search of new compounds with enhanced physical properties. Pulsed laser deposition and co-sputtering serve as the main tools to generate combinatorial thin film library wafers. Various scanning and/or parallel measurement techniques are employed to obtain quantitative mapping of various physical properties across the libraries. Our primary targets are inorganic functional materials such as magnetic materials, piezoelectric materials, and superconductors. We map the structural properties across libraries and quickly cross-reference them with known phases in crystallographic databases. The need for such a study is common among combinatorial investigation of virtually all topics. Automated scanning X-ray diffraction across entire libraries is carried out at a synchrotron beamline as well as with in-house diffractomerers. Machine learning algorithms are used for materials property prediction and materials classification. The algorithms also provide a means for determining latent variables - primary predictors of material structure and properties that might otherwise be buried in the large datasets. Combinatorial investigation guided by theories will also be discussed.

MM 17: Topical Session: TEM-Symposium - HR Imaging & Analytic I

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

Topical Talk MM 17.1 Tue 10:15 H4

Quantification of sample properties by low-energy scanning transmission electron microscopy — Erich Müller, Holger Blank, Marina Pfaff, Tobias Volkenandt, and •Dagmar Gerthsen — Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany

Scanning transmission electron microscopy (STEM) at low energies (< 30 keV) is a promising technique for microstructure analysis and quantification of sample properties. Low-energy STEM images can be taken in a standard scanning electron microscope which is equipped with a STEM detector. Using thin samples a high lateral resolution in the order of 1 nm can be achieved which is sufficient for many materials science and biological applications. Modelling of the STEM image intensity at low electron energies can be performed by Monte-Carlo simulations, which is considerably less complex than STEM image simulations at high electron energies. Quantification of the sample information (local sample thickness and composition) can be performed by comparison of simulated and experimental STEM intensities.

High-angle annular dark-field STEM is particularly interesting because the chemical sensitivity of this particular imaging mode increases with decreasing electron energy. The high chemical sensitivity can be exploited for the study of samples which provide low contrast as, e.g., polymers and biological objects. We will show applications of low-energy STEM in materials science and biology with a particular focus on quantification of the sample thickness and sample composition in compound semiconductors.

MM 17.2 Tue 10:45 H4

Quantitative HAADF-studies on GaP/Si heterostructures — •Andreas Beyer, Nikolai Knaub, Benedikt Haas, Katharina Gries, Katharina Werner, and Kerstin Volz — Structure and Technology Research Laboratory, Philipps-Universität, Marburg, Germany

The growth of III/V-materials on Si enables a variety of new optoelec-

tronic devices. We investigate GaP grown on Si as a model system. The growth of a polar material on nonpolar substrate holds several challenges as the interface is not necessarily charge neutral and antiphase domains (APDs) can form at monoatomic steps of the Si-surface.

High resolution high angle annular darkfield (HAADF) measurements were carried out in a JEOL JEM 2200FS,equipped with a corrector for spherical aberration of the condenser lens system. For quantification of the data HAADF-intensities were simulated using an absorptive potential approach.

The simulated and experimental HAADF-images show that the intensity ratio of Si and GaP is not constant but a function of local TEM sample thickness and microscope parameters. This can be exploited to determine the thickness via high resolution HAADF images of the interface. The determined thickness values are compared to the ones derived by electron energy loss spectroscopy. For a known sample thickness the influence of element intermixing at the interface as well as the local atomic structure of present APDs on the HAADF-intensity is investigated and quantified.

MM 17.3 Tue 11:00 H4

Investigating the potential of determining the 3D structure of nanoparticles from through focus series of HRTEM images — Alexander Surrey[1,2], Darius Pohl[1,2], Ludwig Schultz[1,2], and •Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany. — [2]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

The acquisition of through focus series of HRTEM images allows for a determination of the complex electronic exit wave function (EWF) which is a result of modifications of the incoming electron wave through multiple scattering processes within the sample. On the other hand, using the channeling theory in combination with the vacuum propagator to control the defocus in principle allows for a quantitative reconstruction of the full 3D structure of the specimen from the amplitudes and phases of the EWF through Argand plots. In order to explore the applicabitity of this approach we have calculated the EWF for a 4 nm Au octahedron supported by 5 nm of amorphous carbon by means of a multi-slice algorithm and subsequently back-analysed the likewise obtained EWF with the above mentioned approach to reconstruct the 3D structure of the model particle. We find that such a reconstruction should indeed be possible under ideal microscopy conditions. However, taking into account realistic limitations of the imigang process even for the case of state-of-the-art aberration-corrected microscopy leads to a collapse of the channeling circle thereby impeding an unambiguous reconstruction of the structure. These theoretical findings are confirmed by the results of likewise conducted experiments.

MM 17.4 Tue 11:15 H4

Novel III/V-Alloys Investigated Using Transmission Electron Microscopy — •Tatjana Wegele, Rafael Fritz, Vivien Vossebürger, Kakhaber Jandieri, and Kerstin Volz — Faculty of Physics and Material Science Centre, Philipps-University Marburg, D-35032 Marburg

Three- and four-compound III/V semiconductor layers are a must-have for efficient solar cells. We use boron atoms and/or arsenic atoms as substituents in GaP or GaAs host materials. The incorporation of these atoms allows to grow metastable materials lattice matched on a substrate with a band gap tuned nearly to a desired value. The amount of the incorporated substituents as well as the crystal quality and therefore the efficiency of the semiconductor devices depend on well-optimized growth conditions.

We investigated GaP-based (BGa)(AsP) and (BGa)P as well as GaAs-based alloys using transmission electron microscopy combining the following techniques: Dark-Field Imaging, High-Resolution Imaging, High-Angle Annular Dark-Field Imaging and Energy Dispersive X-ray Spectroscopy. The latter two are used in scanning TEM mode.

We were able to determine the chemical composition of the investigated layers and also to directly test the quality of the interfaces. The maximum possible concentration of incorporated substituent atoms, that do not produce any defects in the layers, was determined. Moreover the homogeneity or inhomogeneity of the substituents distribution in the three- and four-compound layers, respectively, were visualized and quantitatively studied.

MM 18: Computational Materials Modelling - Phase Stability I

Time: Tuesday 10:15–11:30 Location: H24

MM 18.1 Tue 10:15 H24

Stability and superconductivity of Ca-B under pressure — •Sheena Shah[1] and Aleksey Kolmogorov[2] — [1]University of Oxford, UK — [2]Binghamton University - SUNY, USA

In the search for MgB_2-like phonon-mediated superconductors, we have carried out a systematic DFT-based evolutionary crystal structure search of the whole Ca_xB_{1-x} system at gigapascal pressures. A set of diverse ground state boron structures are identified for CaB, CaB_2, CaB_4 and CaB_6. The monoboride is predicted to be superconducting at 5 K. Others are predicted to be superconducting at lower temperatures, demonstrating the inverse correlation between thermodynamic stability and superconducting properties. Finally, structural rules have been established for the thermodynamic stability of these alkaline earth metal borides with pressure. For example, we show that ThB_4-type CaB_4 is stable at ambient pressure since the ionic radius of Ca^{2+} is an ideal fit for the boron network.

MM 18.2 Tue 10:30 H24

A joint DFT and experimental study of the competing phases of Calcium at high-pressures and low-temperatures — •Deepa Kasinathan[1], Carina Boerrnert[1], Michael Hanfland[2], Jens Hunger[1], Helge Rosner[1], and Ulrich Schwarz[1] — [1]MPI CPfS-Dresden — [2]ESRF, Grenoble

One of the most unanticipated developments in superconducting critical temperatures (T_c) in the past decade has been the achievement of much higher values of Tc in elemental superconductors by the application of high pressure. Surprisingly, these superconducting states evolve from simple metals that are non-superconducting at ambient pressure. Calcium undergoes a series of structural changes under pressure and superconducts with a T_c as high as 26 K near 160 GPa. There has been a long standing discrepancy among and between various experiments and as well as density functional theory based calculations to correctly identify the various high-pressure phases in calcium. Here, we report on a combined experimental and theoretical work on the multitude of structural phase transitions observed at low-temperatures and high-pressures. In our study, we have performed high-pressure X-ray diffraction experiments at the ESRF synchrotron beam-line (ID09A) to examine, verify and validate the complex phase diagram of calcium.

MM 18.3 Tue 10:45 H24

Crystal structure prediction and electronic properties of Li-based ternary compounds — •Maia G. Vergniory[1], Miguel A. L. Marques[2], Silvana Botti[2], Max Amsler[3], Stefan Goedecker[3], Irais Valencia[2], Antonio Sanna[1], Evgueni V. Chulkov[4], Arthur Ernst[1], Aldo H. Romero[1], and Eberhard K. U. Gross[1] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [2]Universite de Lyon, F-69000 Lyon, France and LPMCN, CNRS, UMR 5586, Universite Lyon 1, F-69622 Villeurbanne, France — [3]Department of Physics, Universitaet Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [4]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

On the basis of ab initio first principles and using the Minimal Hopping Algorithm we predict the crystal structure of non synthesized LiYZ (Y=Au,Ag, Z=Te,Se) based ternary compounds. We find that, as distinct from expectation, the crystal structure depends strongly on the composition, thus every compound belongs to a different symmetry group and has complexly different electronic properties. We will analyze the fundamental physics below these features considering the calculated ground state structure.

MM 18.4 Tue 11:00 H24

The effect of partial occupancies on lithium ion diffusivity in lithium titanate oxides — •Benedikt Ziebarth — IAM, Karlsruhe Institute of Technology, Kaiserstrasse 12, 76131 Karlsruhe, Germany — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany

The effect of partial occupancies on lithium ion diffusivity in lithium

titanate oxides Lithium titanate oxide (LTO) is a promising candidate as an anode material in future generations of lithium ion batteries. In this work, we investigate the diffusion barriers for lithium ions in two different crystal structures of LTO using the density functional theory. Our calculations show that the activation barriers vary between $0.30-0.48\,\mathrm{eV}$ for the spinel phase $Li_4Ti_5O_{12}$ and between $0.20-0.51\,\mathrm{eV}$ in the lithiated rock salt phase $Li_7Ti_5O_{12}$. The origins of the rather broad ranges of activation energies are related to different chemical environments of the diffusion channels due to partial occupancies of some sites in LTO. Our results reveal that determination of lithium diffusion constants in LTO cannot be carried out by using a single activation barrier. Instead, the local chemical environment of the diffusion paths must be considered to correctly capture the variety of activation barriers.

MM 18.5 Tue 11:15 H24

Prediction of a hybrid graphene-diamond like phase — •Silvia Bahmann, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany

The crystal structure contains the most important information about a crystalline solid. Therefore, predicting it from first principles by just specifying the chemical composition has been long pursued. Increasing computer power in the last decade made it possible to explore the huge search space ($3N+3$ dimensions where N is the number of atoms) of unknown crystal structures using density functional theory.

We applied an evolutionary strategy that uses the main features of natural evolution namely recombination, mutation, selection and the survival of the fittest and found a new hybrid graphene-diamond like phase. Our structure can be described as crossing graphene sheets that form nearly rectangular tubular pores. The atoms at the crossing lines show nearly perfect tetrahedral coordination whereas the ones in between exhibit sp^3 bonding. Crossed graphene is shown to be dynamically stable with respect to phonons and elastic constants. The latter also point out the close relation to graphite/graphene. By inspecting the eletronic structure similarities to graphene also become visible.

MM 19: Topical Session: Combinatorial Materials Science I

Time: Tuesday 10:15–11:30 Location: H25

Topical Talk MM 19.1 Tue 10:15 H25

Development of new materials using high-throughput thin film experimentation and up-scaling — •Alfred Ludwig — Ruhr-Universität Bochum, Germany

New or optimized multifunctional materials are needed, e.g. for miniaturization of technological products with improved functionality even in extreme conditions or for efficient production/storage/conversion of energy carriers. For the discovery and optimization of new materials combinatorial and high-throughput experimentation methods are very effective. The materials to be investigated are deposited in the form of materials libraries by special magnetron sputter deposition methods (co-deposition, wedge-type multilayer deposition, shadow masking). These materials libraries are subsequently processed and characterized by high-throughput experimentation methods (automated EDX, XRD, temperature-dependent resistance and stress screening) in order to relate compositional information with structural and functional properties. The talk will cover examples of the combinatorial development of intermetallic materials for shape memory (Ni-Ti-X-Y, Fe-Pd-X) applications as well as new materials for solar water splitting. The obtained results are visualized in the form of composition-function diagrams. Examples of up-scaling from thin film findings to bulk applications are discussed.

Topical Talk MM 19.2 Tue 10:45 H25

A combinatorial approach to the synthesis of novel oxide and oxinitride thin films — •Michael Stüber, Stefanie Spitz, Harald Leiste, and Sven Ulrich — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-AWP), 76344 Eggenstein-Leopoldshafen, Germany

The development of new oxide and oxinitride thin films for engineering applications is attracting enormous interest. Besides theoretical modelling of structural design and properties of such materials the systematic evaluation of plasma-based deposition routes towards their synthesis will contribute to create a substantial data base for future material development.

An experimental combinatorial approach to the synthesis of oxide and oxinitride thin films in the systems Al-Cr-O-N and Cr-Zr-O-N will be presented. The thin films were deposited by reactive r.f. magnetron sputtering at 500 °C and 500 W r.f. target power under systematic variation of the reactive gas flows. Thin films with five different compositions were obtained in one deposition process by using a segmented Al:Cr or Cr:Zr sputtering target.

Under specific conditions, (Al,Cr)2O3, (Cr,Zr)2O3, (Al,Cr)2(O,N)3 and (Cr,Zr)2(O,N)3 films are grown in single-phase solid solution corundum-type crystal structure. The microstructure formation and phase stability will be discussed versus composition, pressure and the impact of nitrogen gas flow. It will be shown that the oxinitride materials can exhibit superior mechanical properties compared to the oxide materials.

MM 19.3 Tue 11:15 H25

Microstructure formation of magnetron sputtered Cr-V-O thin films in dependance of chemical composition — •Stefanie Spitz, Michael Stüber, Harald Leiste, and Sven Ulrich — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-AWP), 76344 Eggenstein-Leopoldshafen, Germany

The system Cr-V-O is of interest for the development of novel oxide thin films due to the ability of Cr and V to build the corundum-type structure if the oxygen supply is sufficient. Utilizing a combinatorial approach for thin film synthesis in magnetron sputtering, different Cr-V-O coatings with a wide range of compositions from Cr-rich to V-rich could be deposited in one process. An r.f. power of 500 W was applied at a segmented Cr-V target. The substrate temperature was 350 °C. The total gas pressure was kept constant at 0.4 Pa. Additionally, a substrate bias voltage up to -100 V was applied.

The elemental composition was analysed by EPMA. For thin films sputtered with 0 V bias Cr:Zr ratios of 7.4, 2.0 and 0.6 were obtained. The metal:non-metal concentration ratio shifted from 2:3 (for Cr-rich coatings) to about 2:5 (for V-rich coatings). XRD analyses indicate a nanocrystalline $(Cr,Zr)_2O_3$ solid solution in corundum-type structure for a Cr:Zr ratio of 7.4. The coatings with the highest Zr content were X-ray amorphous. Applying only a small bias voltage almost doubles the hardness values to maximum 21 GPa.

MM 20: Transport & Diffusion I

Time: Tuesday 10:15–11:30 Location: H26

MM 20.1 Tue 10:15 H26

Temperature dependent structure transition of a Σ17 (410) grain boundary in copper investigated by the radiotracer technique — •Henning Edelhoff[1], Harald Rösner[1], Sergei Prokofjev[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Russia

Due to the increasing amount of grain boundaries in fine- and ultra fine-grained materials, the effect of interfaces on materials properties is of great importance. Still the fundamental understanding of grain boundaries and their energy, structure and kinetics as a function of temperature and solute segregation is incomplete. A promising method to gain the information about kinetics and structure is to use the radiotracer technique with individual well characterized grain boundaries.

In the previous work on Ag diffusion in a Cu grain boundary of "near Σ5 (310)"-type, a structural transition of the grain boundary was observed at approximately 850 K, which also appears in MD simulations.

To take a closer look on possible structure transitions within interfaces, a Σ17 tilt grain boundary is investigated in the temperature range from 714 K to 952 K. The grain boundary diffusion of 110m-Ag in a Cu Σ17(410) bi-crystal is measured along the misorientation axis and the results are interpreted on the basis of TEM and MD simulation.

MM 20.2 Tue 10:30 H26

Formation and growth of Cu3Si studied by SNMS — •Zoltán Balogh[1], Mohammed Ibrahim[1], Guido Schmitz[1], Bence Parditka[2], and Zoltán Erdélyi[2] — [1]Westfälische Wilhelms Universität-Münster Wilhelm Klemm Straße 10, Münster, D-48149 (Germany) — [2]University of Debrecen PO Box. 2, Debrecen, H-4010 (Hungary)

Metal induced crystallization is one of the methods to reduce the crystallization temperature of amorphous Si films [1]. This can happen either by the bond weakening effect of eutectic forming materials or by assistance of metal-silicide template. Metal-Si solid state reactions also represent some of the very few examples in which a linear kinetics in the formation of an intermetallic layer is observed [2,3].

We investigated the formation and the subsequent growth of the Cu/Si reaction layer in sputter deposited thin films. Bilayers comprising 45 nm Cu on 120 nm a-Si were deposited upon Si <100> substrates and annealed at 135 °C under high vacuum conditions. XRD revealed that Cu3Si does grow as a result of the annealing. By SNMS and XPS investigations we found that (i) the Cu3Si layer is not present in the as-deposited layer, (ii) a 20 nm thick layer is quickly formed after very short annealing and that (iii) further growth appears linearly with significantly slower rate of 1 nm/h.

[1] Z. Wang et al., Adv. Eng. Mater., 11 (2009) 131.
[2] F.M. d'Heurle and P. Gas, J. Mater. Res., 1 (1986) 205.
[3] F. Nemouchi et al., Appl. Phys. Lett., 86 (2004) 041903.

MM 20.3 Tue 10:45 H26

Growth kinetics and interface structure of copper silicides studied by atom probe tomography — •Mohammed Ibrahim, Zoltán Balogh, Patrick Stender, Mohammed Reda Chellali, and Guido Schmitz — Westfälische Wilhelms Universität-Münster Wilhelm Klemm Straße 10, Münster, D-48149 (Germany)

The production of crystalline Si films is important for numerous applications. In contact with some silicide forming components, the crystallization temperature of amorphous Si is significantly reduced [1]. Si deposited on Cu is also considered as a possible anode for high capacity Li-ion batteries. Solid state reaction between the Si and the Cu current collector results in the formation of copper-silicides [2]. Gaining information on the kinetics of this reaction is thus desired for many applications.

We investigated the early phases of the growth of Cu-silicides by laser assisted APT [3]. Cu and Si have been deposited upon field developed tungsten (W) tips. We found that an intermixed zone is already formed during the deposition. Its thickness strongly depends on the stacking order. The transition zone is broad in the case of Cu on Si and much sharper for Si on Cu. After annealing at 130 °C (from 30 min to 4 hours) we observe formation of a Cu3Si layer with few tens of nm thickness. Remarkably Si segregates to the free surface and to the Cu/Cu3Si interface.

[1] Z. Wang et al., Adv. Eng. Mater., 11 (2009) 131.
[2] H. Chen et al., J. Power Sources, 196 (2011) 6657.
[3] R. Schlesiger et al., Rev. Sci. Instrum., 81 (2010) 043703.

MM 20.4 Tue 11:00 H26

Solute diffusion along interfaces in nanocrystalline copper — •Matthias Wegner[1], Jörn Leuthold[1], Martin Peterlechner[1], Xiaoyan Song[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Beijing University of Technology, 100124 Beijing, China

Diffusion of solutes along interfaces in nanocrystalline copper with grain sizes of about 40 and 50 nm produced by Spark Plasma Sintering (SPS) is investigated by means of the radiotracer technique. The small grain size in addition to the good thermal stability of SPS Cu yields a unique opportunity to measure radiotracer diffusion in a nanocrystalline material without complicating effects like grain boundary motion, grain growth or recrystallization. Diffusion measurements were done within the temperature regime of 435 K up to 470 K. The results are discussed with respect to a potential influence of triple junction diffusion on the measured diffusion profiles. Possible mechanisms which may be responsible for stabilizing the microstructure of the nanocrystalline copper up to temperatures of ˜ 1/3 of the melting temperature are elucidated. Furthermore the amount of porosity and its effect on the measurements is discussed. As a main result, the absence of a size dependence of the specific grain boundary diffusion rate is observed.

MM 20.5 Tue 11:15 H26

Experiments on the Investigation of Self-Diffusion in Amorphous Silicon — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

A key task in material science is the investigation of self-diffusion in solids in order to characterize kinetic processes and to identify point defects and process relevant activation energies. In spite of its technological importance, e.g. in photovoltaic cells, there are no experimental data in current literature on the self-diffusion in amorphous silicon (a-Si). This is mainly due to a combination of the expected low diffusivities and the intrinsic metastability of a-Si in the accessible time and temperature range. In order to determine self-diffusivities $^{29}Si/^{28}Si$ isotope multilayers are prepared by ion-beam sputtering. Afterwards those samples are thermally treated in Ar atmosphere at different temperatures below the crystallization limit in order to induce diffusion. The isotope multilayers are amorphous and chemically homogeneous (as shown by TEM and XRD) but isotope-modulated. Consequently diffusion can be measured by time-of-flight neutron reflectometry, a method capable of determining extremely small diffusion lengths in the order of 1 nm and below [1,2]. First results point to an onset of diffusion at about 350 °C. The influence of O impurities on structure and diffusion is discussed.

[1] H. Schmidt et al.; Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104

MM 21: Topical Session: TEM-Symposium - HR Imaging & Analytic II

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

MM 21.1 Tue 11:45 H4

Energy dispersive X-ray spectroscopy using silicon drift detectors in TEM; state and prospects — •Meiken Falke — Bruker Nano GmbH, Berlin, Germany

Energy dispersive X-ray spectroscopy (EDS) in the electron microscope uses characteristic X-rays for element identification, which are generated during the interaction of electrons with the sample. To detect a suitable amount of the X-rays generated by a small amount of matter is a challenge for EDS technology. Measures such as low dose techniques or low voltage and the demand for very fast analysis make the problem even more complicated. One part of the solution is to increase the solid angle for X-ray detection. Various approaches have been implemented. The better a sphere around the sample can be resembled, the more X-rays can be captured. Data from single and multiple chip EDS systems will be presented. Another solution for chemical analysis on the nanoscale and below is to combine the EDS-system development with adjustments in pole piece and EDS port geometry as well as in beam current quality and sample holder design. We will demonstrate that this approach can enable a solid angle of up to 1sr but also single atom X-ray spectroscopy even at a relatively low solid angle of 0.1sr using 60keV accelerating voltage to avoid radiation damage in graphene [1].

[1] T. C. Lovejoy et al., Appl. Phys. Lett.100, 154101 (2012).

MM 21.2 Tue 12:00 H4

Electron microscopy study of Y-doped BSCF — •Matthias Meffert[1], Philipp Müller[1,3], Heike Störmer[1], Christian Niedrig[2], Stefan F. Wagner[2], Ellen Ivers-Tiffée[2,3], and Dagmar Gerthsen[1,3] — [1]Laboratorium für Elektronenmikroskopie, KIT, Karlsruhe, Germany — [2]Institut für Werkstoffe der Elektrotechnik, KIT, Karlsruhe, Germany — [3]DFG Center for Functional Nanostructures, KIT, Karlsruhe, Germany

Mixed ionic-electronic conducting ceramic membranes are well suited for oxygen separation. The cubic phase of perovskite $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF) has received particular attention due to its high oxygen permeability. However long-term phase stability at application relevant temperatures (700 - 800 °C) is still an issue to be solved. Oxidation of the B-site cation cobalt and a concurrent decrease of ion radius cause a slow decomposition of the cubic BSCF phase. Beside the hexagonal phase precipitates with plate-like morphology are formed which consist of a mixture of different phases.
To improve the stability of the cubic BSCF phase doping with yttrium was investigated using analytical transmission electron microscopy and scanning electron microscopy. Y-doping suppresses the formation of cobalt oxide precipitates which serve as nucleation centers for plate-like precipitates and the hexagonal phase in undoped BSCF. Hence, the hexagonal phase is only formed at grain boundary triple points (800 °C) and decorates most grain boundaries at 700 °C. Samples annealed at elevated temperatures (≥900 °C) are free of secondary phases in contrast to undoped material.

MM 21.3 Tue 12:15 H4

Understanding magnetic domains of Ni-Mn-Ga films by TEM — •Christian Behler[1,2], Karin Vogel[3], Daniel Wolf[3], Sebastian Sturm[3], Anett Diestel[1], Anja Backen[1], Ludwig Schultz[1,2], Hannes Lichte[3], and Sebastian Fähler[1,2] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany — [3]Triebenberg Laboratory, Institute of Structure Physics, Technische Universität Dresden, 01062 Dresden, Germany

Due to the high strain up to 10% magnetic shape memory alloys are of particular interest for magnetic microactuators. On the surface of suitable epitaxial, 14M modulated Ni-Mn-Ga films a magnetic stray field contrast perpendicular to twin boundaries is observed by means of magnetic force microscopy [1]. However, different domain configurations are suggested to result in such a stray field image. To determine the real magnetic domain structure within the whole films first several crosscuts of two different orientations were prepared using focused ion beam milling. Then the micromagnetic structure of these lamellas were studied using lorentz microscopy (fresnel imaging mode) and off-axis electron holography. As result we observe a magnetic domain pattern, in which the direction of magnetization follows the magnetic easy axis (c_{14M}) as well as containing 180° domain walls within one variant. This work is supported by SPP 1239, www.MagneticShape.de.
[1] Anett Diestel et. al., Scripta Mat. 67 (2012),423-426

Topical Talk MM 21.4 Tue 12:30 H4

Surface plasmon coupling studies through near-field mapping of electromagnetic modes in electron microscopy — Burcu Ögüt[1], Nahid Talebi[1], Wilfried Sigle[1], Ralf Vogelgesang[2], and •Peter A. van Aken[1] — [1]Stuttgart Center for Electron Microscopy, Max-Planck Institute for Intelligent Systems, Stuttgart, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Miniaturization technology in optics has become an emerging field with the aim of overcoming the obstacle of the diffraction limit of light. Plasmons which are coherent collective oscillations of quasi-free electrons in a metal volume or surface provide exciting new options for information transfer in channels smaller than this diffraction limit. This presentation concentrates on different plasmonic phenomena which are observed in a TEM in combination with EELS and EFTEM. Plasmonic coupling behaviour of electromagnetic fields at metallic nano-structures were investigated. The experimental results are cross-checked by different simulation techniques based on discrete dipole approximation, finite element method, and 3D finite-difference time-domain methods unveiling the precise electromagnetic field distribution. The hybridization of electromagnetic fields of closely spaced rectangular nanoslits was analysed in the framework of Babinet*s principle, and the presence of toroidal modes in a metal ring formed by an oligomer of holes was demonstrated for the first time. Resonant wedge plasmon modes in a triangular nanoprism were observed, and symmetry breaking concepts are thoroughly discussed.

MM 22: Computational Materials Modelling - Phase Stability II

Time: Tuesday 11:45–13:00 Location: H24

MM 22.1 Tue 11:45 H24

Stability analysis of complex phases in transition-metal alloys with analytic bond-order potentials — •Thomas Hammerschmidt and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Topologically close-packed (TCP) phases play in important role for precipitate hardening in steels and as detrimental brittle phase in single-crystal superalloys. The structural stability of TCP phases can be attributed to an interplay of band-filling effects and differences in atomic size. In order to further understand this interplay, we apply a hierarchy of electronic-structure methods: On the level of density-functional theory (DFT), we determine the formation energies of the TCP phases A15, sigma, chi, mu, C14, C15 and C36 in the binary systems Ta-V/Nb, Re-V/Cr/Nb/Mo, and Co-V/Cr/Nb/Mo. The binary structures as obtained from relaxations by DFT are then analyzed on the basis of a simple canonical tight-binding (TB) model that provides a coarse-grained description of the electronic structure. The solution of the tight-binding problem is computed within the formalism of analytic bond-order potentials (BOPs) as a second coarse-graining step. This enables us to decompose the binding energy in contributions from different neighbor shells in terms of moments of the electronic density-of-states obtained from analytic BOP. We analyze the importance of internal relaxations in the DFT-relaxed structures across the transition metals series for elemental TCP phases. Furthermore we discuss the identification of size effects in binary TCP phases obtained from DFT calculations in terms of moments from analytic BOP.

MM 22.2 Tue 12:00 H24

Structural stability of topologically close-packed phases in the Fe-Nb system — •Alvin Noe Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Germany

The amount of refractory metals in powder metal steels is limited by carbide formation during atomization of the powder. Diffusion alloying makes it possible to push this limit by starting from a carbon-free melt. This route leads to the formation of topologically close-packed (TCP) phases which are transformed into carbides by subsequent addition of graphitic carbon during powder consolidation. In order to optimize this new processing method, one has to determine the properties of the observed TCP phases and to understand the mechanism of TCP-carbide transformation. In this study, we employ density functional theory (DFT) to determine the stability of TCP phases in the Fe-Nb system. The TCP phases that we considered include the A15, Laves(C14,C15 and C36), χ, μ and σ. Each of the Wyckoff positions were filled with either Fe or Nb allowing us to change the composition of the binary system. According to our calculated values of the heat of formation, the Laves phases and the μ phase are stable with stoichiometric compositions of Fe_2Nb and Fe_7Nb_6, respectively. For the Laves phases we observe a very close competition with the heats of formation differing only by a few meV. Our calculations also suggest a broad stability range for the μ phase extending up to approximately 54 at % Nb. Our findings are consistent with the experimental phase diagram of the Fe-Nb system. In addition, we also determined the influence of C defects on the stability of the Laves and the μ phases.

MM 22.3 Tue 12:15 H24

A cluster-expansion Hamiltonian for the modeling of phase stabilities in the Ni-rich Ni-Al alloy — •Sascha B. Maisel, Michaela Höfler, and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Denickstrasse 15, Building K, 21073 Hamburg, Germany

Binary NiAl forms a well known stoichiometric phase called the γ'-Phase at 25 at. % Al. This phases shows a pronounced $L1_2$ ordering tendency and its precipitates are popular hardeners in many advanced alloys. Effective cluster-expansion interactions for the binary NiAl system between 0 and 25 at. % Al are needed as part of a larger project, which ultimately aims to supply model-Hamiltonians for multicomponent Ni-based super alloys. We have parametrized such an effective Hamiltonian for the Ni-rich Ni-Al alloy and present it in this talk, along with benchmarks of its efficiency and its accuracy in predicting formation enthalpies and phase boundaries when compared to both DFT input and experiments.

MM 22.4 Tue 12:30 H24

Ab-initio study of kappa-carbide precipitates in an austenitic Fe matrix — •Poulumi Dey, Roman Nazarov, Martin Friak, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

The quaternary system Fe-Mn-Al-C exhibits interesting physical properties and is highly relevant for a new class of steels with high strength and toughness. Depending on the composition, experiments show the precipitation of kappa-carbides, (Fe,Mn)3AlC in these steels, which significantly influence the microstructure. In order to theoretically predict the formation of these precipitates, we perform a thorough investigation of the structure, composition and magnetism of kappa-carbides in an austenitic Fe-based matrix with the aid of density functional theory. The formation energy of kappa-carbides is computed as a function of the chemical potentials of its constituents, including the effect of different magnetic structures. For both aspects the constraints posed by an austenitic Fe-Mn-Al matrix have been taken into account. Our results show that the Mn-free Fe3AlC is energetically most favorable over a wide range of chemical potentials and hence most abundant as coherent precipitate in the matrix. An increase in Mn concentration results in a monotonic increase in the lattice constant of kappa-carbides and therefore a growing lattice mismatch between the kappa-carbide and the matrix. The results can be used to design strategies to adjust the amount of kappa-carbides in Fe-Mn-Al steels.

MM 22.5 Tue 12:45 H24

Comparison of Analytic and Numerical Bond-Order Potentials for bcc Refractory Metals — •Miroslav Cak, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

A systematic coarse-graining of the electronic structure leads from DFT to tight-binding and to bond-order potentials (BOP). The calculation of the total energy of a system of interacting atoms can be carried out within the formalism of either analytic or numerical BOP. Recently, we developed parameterizations of analytic BOPs for the refractory metals Tungsten, Molybdenum, Niobium and Tantalum. These refractory metals play an important role as strengtheners of nickel- and cobalt-based superalloys. Here we employ our new parameterizations in a detailed comparison of numerical and analytic BOP and find very good agreement for various bonding configurations. Comparing these BOP calculations to corresponding first-principles, tight-binding and experimental results confirms the transferability of both BOP schemes to atomic structures encountered in lattice defects. As an application of our BOPs we determine the interaction of dislocations with other defects like vacancies.

MM 23: Topical Session: Combinatorial Materials Science II

Time: Tuesday 11:45–13:00 Location: H25

Topical Talk MM 23.1 Tue 11:45 H25

A combinatorial materials science approach to the development of new functional thin film materials — •Ulf Jansson[1], Fang Mao[1], Tomas Nyberg[2], Urban Wiklund[2], and Mattias Klintenberg[3] — [1]Department of Chemistry-Ångström, Uppsala University, Sweden — [2]Department of Engineering Science, Uppsala University, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

Combinatorial materials science (CMS) enables a rapid discovery of new materials for various applications. Compared with conventional methods, CMS is a powerful tool for time-saving development of new materials. This paper will present a platform for CMS including rapid methods for theoretical modelling, sputtering of gradient films, analysis equipment as well as tools to evaluate mechanical, tribological and electrical properties.

Two examples of screening for new materials will be presented. The first is rapid theoretical screening of M-B-C materials (M=early transition metal) for wear-resistant coatings where new phases based on e.g. tungsten give improved properties. The other example is sliding electrical contacts which must combine low resistivity and contact resistance with low wear rate and friction and high corrosion resistance, a combination of properties which is very difficult to meet simultaneously. We have initiated studies of Ag-based alloys, Ag-M-X, (M and X = selected metals and nonmetals) and with CMS demonstrated that addition of Al together with other metals can increase hardness and reduce friction but still maintain good electric properties.

MM 23.2 Tue 12:15 H25

Polyhedron-based structure maps for pd-bonded systems — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Structure maps are an approach to identify the governing factors that determine whether a mixture of elements will form a compound and which crystal structure is to be expected. Here, we present new structure maps for the pd-bonded systems that are footed on databases of experimentally observed structures. Our new structure maps depend on atomic properties and on the local environment of the crystallographic Wyckoff sites. The latter is determined by a polyhedron analysis that decomposes the atomic environment into corresponding coordination polyhedra. This enables us to identify trends in the favorite coordination number and relationships between the global compound and the local coordination polyhedron composition for the p-block elements. The information from the polyhedron analysis enters the order parameters that represent the axes of the structure maps. As a result, we find very good separation between different crystal structures. The chosen order parameters are also able to account for fractionally occupied Wyckoff sites.

MM 23.3 Tue 12:30 H25

Oxygen Incorporation in Cr2AlC Investigated by Combinatorial Thin Film Synthesis and X-Ray Stress Analysis — •Lin Shang, Moritz to Baben, Jens Emmerlich, and Jochen M. Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

The oxygen incorporation in Cr2AlC was studied by combinatorial thin film synthesis. Thin films with chemical concentration gradient were deposited by DC magnetron sputtering from elemental targets, and oxygen was intentionally introduced. Ab initio calculation results indicate that oxygen is incorporated interstitially in the Al layer of Cr2AlC, even for carbon-deficient Cr2AlC. Two phase-regions of Cr2AlC and Cr2Al were investigated in order to study oxygen incorporation in carbon-deficient Cr2AlC. X-ray stress analysis data indicate that the a and c lattice parameters increase with increasing oxygen content. These trends are in good agreement with the change in lattice parameters predicted by ab initio calculations and therefore corroborates the notion of interstitial oxygen incorporation in Cr2AlC. A metastable solubility limit for oxygen of 3.5 at% was determined. This is the first report on interstitial oxygen incorporation in MAX phases and may be of relevance to the initial stages of oxidation.

MM 23.4 Tue 12:45 H25

Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals — Li-Fang Zhu[1], •Martin Friak[1], Helge Fabritius[1], Pavlina Hemzalova[1], Andreas Ziegler[2], Svetoslav Nikolov[3], Anna Janus[1], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]University of Ulm, Ulm, Germany — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria

We employ ab initio calculations and investigate the single-crystalline elastic properties of $(Ca,Mg)CO_3$ crystals covering the whole range of concentrations from pure calcite $CaCO_3$ to pure magnesite $MgCO_3$.

Studying different distributions of Ca and Mg atoms, our theoretical results show that the energetically most favorable configurations are characterized by elastic constants that nearly monotonously increase with the Mg content. Based on the first principles derived single-crystalline elastic anisotropy, the integral elastic response of $(Ca,Mg)CO_3$ polycrystals is determined employing a mean-field self-consistent homogenization method. As in case of single-crystalline elastic properties, the computed polycrystalline elastic parameters sensitively depend on the chemical composition and show a significant stiffening impact of Mg atoms on calcite crystals in agreement with experimental findings.

MM 24: Transport & Diffusion II

Time: Tuesday 11:45–13:00 Location: H26

MM 24.1 Tue 11:45 H26

Diffusion and microhardness in ultrafine grained nickel produced by high-pressure torsion — •Simon Trubel, Sergiy Divinski, Martin Peterlechner, Gerrit Reglitz, Jörn Leuthold, Matthias Wegner, Christian Simon, and Gerhard Wilde — Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Ultrafine grained and nanocrystalline materials produced by methods of severe plastic deformation have roused a growing interest in science and technology due to their unusual property combinations. Here, tracer diffusion is used as a sensitive probe to determine how the internal interfaces in a material are affected by severe deformation. Nanoindentation was applied to obtain information about the local mechanical properties of the material and their evolution with annealing temperature. EBSD (electron backscatter diffraction) and TEM (transmission electron microscopy) were utilized for microstructure examination. Nickel material of 99.6 wt. % purity was subjected to high pressure torsion (HPT), performing several rotations under a quasi-hydrostatic pressure of 2 GPa. By this treatment, ultrafine grained Ni is produced. Subsequently, grain boundary self-diffusion was measured at several temperatures applying the radioactive isotope 63Ni. The measurements indicate that the specific grain boundary diffusivity is significantly enhanced. The results of the complementing methods are discussed in the context of grain boundary structure modifications through severe plastic deformation.

MM 24.2 Tue 12:00 H26

Thermal stability of fast diffusion pathways in ECAP-deformed Ag — •Jochen Fiebig[1], Sergiy Divinski[1], Werner Skrotzki[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Structural Physics, Dresden University of Technology, Dresden, Germany

We performed a systematic study of grain boundary self-diffusion in ultrafine grained silver produced by equal channel angular pressing (ECAP) using the radiotracer method (^{110m}Ag-tracer solution) in combination with parallel sectioning by microtome slicing. The grain boundary diffusion was measured depending on the deformation state and the resulting profiles unambiguously revealed the existence of grain boundaries with enhanced excess energy density, i.e. 'high-energy' grain boundaries. Based on this result, we focused on the thermal stability of these specific grain boundaries. Therefore, the diffusion properties after different heat treatments were studied and the microstructure was analyzed with respect to structural elements that survived the heat treatment. Additionally, calorimetric measurements were performed. Applying Borisov's formalism [1] the excess energy of high-energy grain boundaries was determined. The energy of general high-angle grain boundaries was measured to be about 0.5 J/m^2. The grain boundary energy of high-energy grain boundaries is about 10 % to 20 % higher.

[1]V.T. Borisov, V.T. Golikov, and G.V. Shcherbedinsky, Phys. Metall. Metallogr. 17, 881 (1964)

MM 24.3 Tue 12:15 H26

Effect of UFG structure on grain boundary diffusion in an Al-Mg-Sc-Zr alloy produced by ECAP — •Anna Mogucheva[1,2], Sergiy Divinski[2], Rustam Kaibyshev[1], and Gerhard Wilde[2] — [1]Belgorod State University, Pobeda 85, Belgorod, 308015, Russia — [2]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

An aluminum alloy 5024 (Al-4.6%Mg-0.35%Mn-0.2%Sc-0.09%Zr) was subjected to equal channel angular pressing (ECAP) with the back pressure of 20% ram pressure using rectangularly shaped channels. Processing to the strain of 8 at a temperature of 300oC resulted in the formation of a fully recrystallized structure with a grain size of $1\mu m$. The kinetic properties of grain boundaries after this treatment were investigated by the radiotracer technique using the 65Zn isotope. The impact of the microstructure on the mechanical properties at elevated temperatures and on the mechanisms of grain boundary diffusion is discussed in detail. A correlation between the superplastic behaviour of the 5024 aluminum alloy and the diffusion properties of the interfaces is also analysed.

MM 24.4 Tue 12:30 H26

Contact resistance and field effects of graphene field effect transistors probed by Kelvin Probe Force Microscopy — •Carlos Alvarado[1], Gerd Bacher[1], Wolfgang Mertin[1], and Daniel Neumaier[2] — [1]Werkstoffe der Elektrotechnik and CENIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]AMO GmbH, 52074 Aachen, Germany

A promising route for large area, high quality graphene sheets suitable for electronic applications is the CVD growth through cooper foils. On its way to become the new material of choice in high frequency electronics, transistors based on CVD grown graphene have to be fabricated and their electrical properties have to be understood on a microscopic scale.

Here, back gate field effects transistors based on CVD grown graphene have been prepared. By spatially resolved Kelvin Probe Force Microscopy (KPFM) on an operating device, the voltage drop profile at the contacts and the potential distribution along the graphene channel are directly measured. Our results show how defects like contaminations or vacancies alter the voltage drop profile and the contact resistance, which is confirmed by 4-probe measurements. We are able to visualize the changes in the potential distribution due to back-gated field effects by KPFM imaging, which opens the possibility to relate the macroscopic I-V characteristics with the distribution of the electrical potential in the device on the nanoscale

MM 24.5 Tue 12:45 H26

Coulomb drag in bilayer graphene — •Jonathan Lux — Institut für theoretische Physik, Universität zu Köln

Coulomb drag measurements provide an interesting possibility to study interaction effects between two adjacent layers. If a current is driven in one of the layers, called the active layer, via Coulomb interaction, momentum can be transferred to the other layer, called the passive layer. This can induce a voltage drop in the passive layer, which can be measured. The ratio of the voltage drop in the passive layer and the current in the active layer is called the drag resistance.

We have calculated the drag resistivity in bilayer graphene (BLG) using Boltzmann kinetic theory, taking into the relevant mode for both particles and holes in each layer. In the Fermi liquid (FL) regime of BLG, the drag resistivity is, up to numerical prefactors, identical to the one in the 2 dimensional electron gas, and independent of the impurity configuration.

Near charge neutrality, Coulomb interaction is able to relax the current, due to the particle–hole symmetry of the low energy theory of BLG. This defines a new regime, which is not accessible in FLs. We found that here the result depends on the ratio of the scattering times of Coulomb and impurity scattering. Special attention is paid to the differences and similarities to the drag in monolayer graphene.

MM 25: Topical Session: TEM-Symposium - Structure-Property

Time: Tuesday 15:00–16:00 Location: H4

Topical Talk MM 25.1 Tue 15:00 H4

Modern Transmission Electron Microscopy in Energy Materials Research — •Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg

Energy is an area where materials technology will play an important role in meeting the needs of the future. Due to the growing importance of environmental issues energy generation, conservation and storage will continue to be major drivers for materials technology. Increasing the efficiencies of energy systems, like solar cells, fuel cells, gas turbines and batteries generally requires the development of new or the improvement of existing materials. Modern transmission electron microscopy (TEM) plays an imporatant role in this process since it provides powerful techniques for investigating the structure, chemistry and defects of materials from the microscale down to the atomic scale and for revealing local structure-property relations. In this presentation examples of the use of modern TEM techniques in energy materials research will be highlighted, including microscopic studies on single-crystal superalloys for turbine engines, transparent electrodes for organic solar cells, porous materials for catalytic gas reactions, and nanoparticle-filled polymers for high voltage electrical isolation.

MM 25.2 Tue 15:30 H4

High-resolution TEM study on carbon nanotubes grown from $Fe_{20}Ni_{80}$ nanoparticles — •Anja Kiessling[1,2], Darius Pohl[1,2], Christine Täschner[1], Mark Hermann Rümmeli[1], Rolf Erni[3], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]TU Dresden, Department of Physics, D-01062 Dresden, Germany — [3]Electron Microscopy Center, Swiss Federal Laboratories for Materials Testing and Research (Empa), CH-8600 Dübendorf, Switzerland

With the aim of studying the interface between the catalyst nanoparticle (NP) and the graphene layers, Carbon Nanotubes (CNT) were grown from $Fe_{20}Ni_{80}$ ("permalloy") NP on silicon substrates. Aberration-corrected high resolution transmission electron microscopy (FEI TITAN^3 80-300) was used to characterize the as-grown CNT.

Recent results obtained with CNT grown from FePt catalyst NP showed an energetically favoured facet for the release of carbon [1]. For the CNT grown from permalloy NP a similar behaviour is predicted from MD simulations and preliminary experimental results are in accord with that. Furthermore, by changing the growth parameters we were able to produce CNT filled with SiC nanowires. These CNT show a strongly distorted lattice. Within a model this behaviour can be explained.

[1] Pohl et al., PRL 107 (2011), 185501.

MM 25.3 Tue 15:45 H4

Electron tomography and HRTEM investigation of PbSe/carbon nanotube hybrid structures for near-infrared photodetectors — •Benjamin Winter[1], Julia Schornbaum[2], Benjamin Butz[1], Jana Zaumseil[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Materials Science Department VII, University of Erlangen-Nuremberg, 91058 Erlangen, Germany — [2]Nanomaterials for Optoelectronics Group, Materials Science Department V, University of Erlangen-Nuremberg, 91058 Erlangen, Germany

Hybrids of single-walled carbon nanotubes (SWNTs) with high charge carrier mobilities and semiconductor quantum dots (QDs) with size-tunable absorption are ideal building blocks for optoelectronic devices. Coupling near-infrared absorbing PbSe QDs to SWNTs transforms the photoexcited states of the QDs into charge separated states. Due to the fast charge transport in SWNTs a dramatic increase of photosensitivity is expected. After the synthesis of the PbSe/SWNT hybrids, Raman spectroscopy indicates that the sp2-carbon lattice of the SWNTs is not chemically modified by the PbSe QDs. This implies that the QDs are attached to the SWNTs without molecular linker and charge transport along the SWNT is not affected. Scanning transmission electron microscopy (STEM) tomography and high-resolution TEM (HRTEM) carried out at 80 kV with an aberration-corrected FEI Titan3 80-300 reveal that the well-defined PbSe QDs partially grow around the SWNT bundles and have a preferred orientation of the {002} lattice planes perpendicular to the longitudinal axis of the SWNT bundles.

MM 26: Computational Materials Modelling - Diffusion & Kinetics I

Time: Tuesday 15:00–16:00 Location: H24

MM 26.1 Tue 15:00 H24

Studying the kinetics of solid-liquid interfaces using transition path sampling — •Daniel Sopu, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The properties of solid-liquid interfaces such as interface energies, interface mobilities and their anisotropy, play an important role in solidification theory. In a first-order phase transformation these interfacial properties determine to a large extent nucleation barriers and growth rates. Depending on the height of the nucleation barrier and the applied driving force, the solidification process can take place on extended time scales which makes it very inefficient to be studied using regular molecular dynamics. Here, we use transition path sampling (TPS) to study the solid-liquid phase transformation in a Lennard-Jones system. TPS is a rare event technique that creates an ensemble of reaction trajectories between two metastable states in phase space. By re-weighting the path ensemble we extract thermodynamic and kinetic properties of the transition and explore the transition mechanisms. In particular we investigate interface free energies, the nucleation and formation of the solid-liquid interface, and anisotropic interface mobilities as a function of temperature.

MM 26.2 Tue 15:15 H24

Effect of local ordering in the melt and at the solid-liquid interface on the growth kinetics in a metallic alloy model — •Mohammed Guerdane[1], Helmar Teichler[2], and Britta Nestler[1,3] — [1]Institute of applied Materials (IAM-ZBS), Karlsruhe Institute of Technology (KIT) — [2]Institute for Materials Physics, University of Göttingen — [3]Institute of Materials and Processes, Karlsruhe University of Applied Sciences

We present a molecular dynamics (MD) study about the structure of a solid-liquid interface between a bcc Zr crystal and a binary NiZr melt. We demonstrate how local atomic order in the liquid phase could transform into a massive lateral ordering at the interface when commensurability is given between the coordination polyhedra of the liquid and the periodic potential of the crystal wall. The influence of this structure on the growth kinetics is quantitatively investigated by linking MD simulations to phase-field modeling. These results contribute to our understanding of the correlation between the stability of the undercooled liquid against crystallization (e.g. in the case of glass forming alloys) and its ability to build up a pronounced atomic order.

MM 26.3 Tue 15:30 H24

Three-dimensional self-learning kinetic Monte Carlo — •Andreas Latz, Lothar Brendel, and Dietrich E. Wolf — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Duisburg, Germany

The reliability of kinetic Monte Carlo (KMC) simulations depends on accurate transition rates. The self-learning KMC method (Trushin et al 2005 Phys. Rev. B 72 115401) combines the accuracy of rates calculated from a realistic potential with the efficiency of a rate catalog, using a pattern recognition scheme.

We expanded the original two-dimensional method to three dimensions (Latz et al 2012 J. Phys.: Condens. Matter 24 485005). Excessive on-the-fly calculations of rates can be avoided by setting up an initial

database, which can be done perfectely in parallel.

The performance is illustrated by applying the method to homoepitaxial growth of Ag on Ag(111) at low temperatures.

MM 26.4 Tue 15:45 H24

Electronic properties and diffusion behavior of Re in Ni-based superalloys: a combined DFT+kMC approach — •Sergej Schuwalow, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

High-temperature mechanical properties of Ni-based superalloys can be significantly improved by adding refractory alloying elements, such as Re, Mo or W. However, due to the complexity of the interplay between composition and microstructure the effect of these additives is only understood in a phenomenological way. Within this work, we investigate the diffusion and segregation behavior of alloying elements in Ni-based superalloys using a combination of *ab-initio* DFT calculations and kinetic Monte Carlo (kMC) modeling, with a particular focus on Re and its interplay with the γ/γ' phase interface. Re is known to be one of the slowest-diffusing elements in Ni [1], and is one of the most effective, and expensive, alloying additives currently in use. In this combined approach, DFT provides insights into local electronic properties of the γ/γ' interface and Re substitutional defects as well as into energetics of microscopic diffusion processes. Based on DFT data, a kMC model is developed to analyze diffusion and segregation behavior of alloying elements on an extended time scale.

[1] M. S. A. Karunaratne, P. Carter, R. C. Reed, Mat. Sci. Eng. A 281, 229 (2000)

MM 27: Topical Session: Combinatorial Materials Science III

Time: Tuesday 15:00–16:00 Location: H25

Topical Talk MM 27.1 Tue 15:00 H25

Bulk Combinatorial Design of nanostructured steels: from composition to mechanisms — Hauke Springer, Ivan Gutierrez-Urrutia, Jae-Bok Seol, Tilmann Hickel, Martin Friak, Jörg Neugebauer, and •Dierk Raabe — Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany

We present an approach to the high-throughput synthesis of bulk nanostructured steels including the variation of composition and thermomechanical processing. This method, referred to as Rapid Alloy Prototyping (RAP), uses semi-continuous high-throughput casting, rolling, heat treatment and sample preparation. The method is demonstrated on a group of Fe-30Mn-1.2C- x Al steels which exhibits a wide spectrum of structural and mechanical characteristics, depending on the respective Al concentration: High amounts of Al additions ($>$ 8 wt.%) resulted in pronounced strengthening, while low concentrations ($<$ 2 wt.%) led to embrittlement of the material during aging. Of specific interest is the formation and high thermal stability of nanoscaled (5-50 nm) kappa - carbides (L1'2). These precipitates appear in the high Al containing alloy variants (e.g. 8%Al) in the form of highly ordered and coherent particles that have nano-sized solid-solution channels between them. Atom probe analysis and electron microscopy (TEM, ECCI) is conducted to better understand the interaction between these nano-precipitates and dislocations. The stability of the kappa carbides and corresponding compositional trends are also studied using ab initio methods.

Topical Talk MM 27.2 Tue 15:30 H25

Combinatorics of RuO2 based thermoelectrics — •Denis Music, Felix Basse, and Jochen Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

RuO2 (P42/mnm, rutile) exhibits interesting transport properties, such as low resistivity, as well as large thermal and chemical stability. It is a promising candidate for thermoelectric devices. The quantum mechanically guided design proposal is based on identifying suitable alloying elements for RuO2 to improve the transport properties and phase stability thereof. Using ab initio calculations, we probed all 4d transition metals and identified Nb and Y to be the best choice. Based on this design proposal, Nb and Y alloyed RuO2 thin films were grown by combinatorial reactive sputtering. Nb and Y can be incorporated in the rutile structure. Nanorods were formed and Nb2O5/Y2O3 coordination appears at increased alloying contents. This may be understood based on our ab initio molecular dynamics data. Surface coarsening on the atomic scale occurs due to O crosslinking of two neighboring Nb-O/Y-O units. Hence, it is reasonable to assume that these units contribute towards the experimentally observed formation of nanorods. Further alloying elements and their influence on structure evolution and transport properties will also be discussed.

MM 28: Transport & Diffusion III

Time: Tuesday 15:00–16:00 Location: H26

MM 28.1 Tue 15:00 H26

^{7}Li NMR field-cycling relaxometry: A powerful tool to investigate lithium ion dynamics in solid-state electrolytes — •Jan Gabriel, Magnus Graf und Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Germany

We use ^{7}Li NMR to study lithium ion dynamics in glasses like (Li_2S)-(P_2S_5) and (Li_2S)-(GeS_2)-(GeO_2). Field-cycling relaxometry is employed in combination with stimulated-echo experiments and line shape analysis to cover a time window extending over 10 orders of magnitude. The stimulated-echo method is suitable to measure the correlation functions $F_2(t)$ of lithium ion dynamics in solids in a time range from 10^{-5} to 10^{1} s. Field-cycling relaxometry measures the spectral density $J_2(\omega)$ from which we obtain a correlation function in a range from 10^{-9} to 10^{-5} s. The motional narrowing of NMR spectra is sensitive from 10^{-4} to 10^{-5} s. These three methods probe translational motion of the lithium ions. The field-cycling and stimulated-echo data revealed a nonexponentiality of the lithium ion dynamics in the studied glasses. The shape of the spectral density $J_2(\omega)$ is well described by a Cole-Davidson function and the decay of the correlation function of $F_2(t)$ is well interpolated by a Kohlrausch-William-Watts function. Observation of the T_1 minimum for a broad range of Larmor frequencies allows us to determine temperature-dependent correlation times and, thus, the activation energy of lithium ion dynamics. When the dynamics of the lithium ions is too slow to be observed at sufficiently low temperatures, field-cycling relaxometry probes the nearly constant loss, which is considered as a universal phenomenon of disordered solids.

MM 28.2 Tue 15:15 H26

Majorana fermions from Landau quantization in a superconductor-topological insulator hybrid structure — •Rakesh P Tiwari[1], Ulrich Zuelicke[2], and Christoph Bruder[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

We show that the interplay of cyclotron motion and Andreev reflection experienced by massless-Dirac-like charge carriers in topological-insulator surface states generates a Majorana-particle excitation. Based on an envelope-function description of the Dirac-Andreev edge states, we discuss the kinematic properties of the Majorana mode and find them to be possible to be tuned by changing the superconductor's chemical potential and/or the magnitude of the perpendicular magnetic field. Our proposal opens up new possibilities for studying Majorana fermions in a controllable setup.

MM 28.3 Tue 15:30 H26

Thermoelectric Transport Coefficients from First Principles — •Karsten Rasim, Christian Carbogno, and Matthias Schef-

fler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, Germany

Significant effort is currently being invested in the search and optimization of thermoelectric (TE) materials, which promise ecologic and economic impact for waste-heat recovery [1]. Respective first-principles studies of the TE transport coefficients have almost exclusively relied on the Boltzmann-transport framework; the electron-phonon coupling is thereby accounted for within first-order perturbation theory [2]. However, such approaches become increasingly questionable at high temperatures due to anharmonic effects and do not allow the assessment of the Seebeck coefficient. The Greenwood-Kubo (GK) method, which includes those effects via *ab initio molecular dynamics*, does not suffer these limitations and provides access to all electronic transport coefficients even at high temperatures. In fact, it has hitherto been used for matter under extreme thermodynamic conditions, e.g, for melts and plasmas [3], but not for condensed materials. We demonstrate and analyze the applicability of the GK method for TE compounds, discuss the required adaptations, the accuracy and the limits of this approach by computing the transport coefficients for direct/indirect band gap semiconductors.

[1] G. J. Snyder and E. S. Toberer, Nature Mat. **7**, 105-114 (2008)
[2] P. Boulet and M. J. Verstraete, Comp. Mat.Sci. **50**, 3 (2001)
[3] V. Recoules and J.-P. Crocombette, Phys. Rev. B **72**, 104202 (2005).

MM 28.4 Tue 15:45 H26

Ab initio study of ionic mobility in anisotropic zirconia — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Electrolytes with high ionic mobility at lower temperatures are the prerequisite for the success of Solid Oxide Fuel Cells (SOFC). One candidate is Yttrium Stabilized zirconia (YSZ). In the past the ionic resistance of YSZ electrolytes has mainly been decreased by reducing their thickness. But this decreases the resistance only linearly. However, the migration barriers of the oxygen ions influence their mobility exponentially. Recently it has been shown that those barriers can be reduced by applying negative [1] or strong positive [2] pressure.

Here we proceed as follows: Since the ionic motion needs to be good in transport direction only, we have freedom in investigating anisotropic structures. And we have found a peculiar one which - according to density functional (DFT) computations, combined with the Nudged Elastic Band (NEB) method and molecular dynamics (MD) computations - has the potential to outperform YSZ.

[1] T. J. Pennycook et al., PRL 104, 115901 (2010) [2] J. A. Hirschfeld and H. Lustfeld, PRB 84, 224308 (2011)

MM 29: Invited Talk (Hauptvortrag): Janisch

Time: Wednesday 9:30–10:00 Location: H24

Invited Talk MM 29.1 Wed 9:30 H24

Modelling and understanding the strength of grain boundaries based on ab-initio results — •Rebecca Janisch — ICAMS, Ruhr-University Bochum

The mechanical properties of interfaces determine the strength and deformability of real microstructures. Key quantities like interface energy, work of separation, theoretical shear and tensile strength are important input parameters for mesoscale-simulations of deformation and fracture. These parameters can be predicted by ab-initio density functional theory calculations with high accuracy. Ab-initio calculations also allow a systematic study of the degrees of freedom, such as interface geometry and chemistry. Unfortunately this parameter-space is very large and ab-initio calculations are extremely time-consuming.

With our studies we are trying to reduce this complexity by looking for correlations between the mechanical properties of grain boundaries. We are investigating whether there is a relationship between grain boundary energy (or grain boundary work of separation) and the theoretical strength of the interface, and furthermore between the shear strength and the tensile strength of grain boundaries. Unfortunately, according to ab-initio results for different material systems and grain boundary geometries, the answer to the first question is no. However, our results display a unique scaling behavior, which greatly reduces the number of parameters that enter the microstructure-property relationship which we are looking for. Furthermore there seems to be a correlation between tensile and shear strength, which will be discussed against the background of existing grain boundary structure models.

MM 30: Topical Session: Fundamentals of Fracture - Modelling Intergranular Fracture

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

MM 30.1 Wed 10:15 H4

Ideal strength of grain boundaries in nickel with segregated sp-impurities — Miroslav Černý[1,2], •Petr Šesták[1,2], Petr Řehák[1,2], Mojmír Šob[1,3], and Monika Všianská[1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty od Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic

Grain boundaries (GB) represent extended planar defects with crucial effect on macroscopic strength of polycrystalline materials. In this first-principles study, we calculate the ideal tensile strength of Σ5(210) tilt GB in nickel under uniaxial loading perpendicular to the GB plane. A computational supercell containing 64 atoms is continually relaxed during the loading. Tensile strength of GB with segregated impurities (S and Al) is compared with that of the clean GB and with the results of previous studies. Differences in computed values demonstrate both the effect of impurities on the ideal strength and the importance of full lattice optimization during the simulation of tensile test.

MM 30.2 Wed 10:30 H4

Structure and stability of vacancies and Cr atoms at Fe Σ5 (210) grain boundary — •Tomasz Ossowski[1], Jan Kuriplach[2], Evgeny Zhurkin[3], Marc Hou[4], and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wrocław, Poland — [2]Department of Low Temperature Physics, Charles University, Prague, Czech Republic — [3]Experimental Nuclear Physics Department, Saint-Petersburg State Polytechnical University, Russia — [4]Physique des Solides Irradiés et des Nanostrucutres CP234, Université Libre de Bruxelles, Belgium

The high-chromium ferritic/martensitic steels are promising materials for advanced reactors. They display high resistance to irradiation induced effects. On the other hand, Fe-Cr alloys serve as a model system to understand microscopic mechanism behind various processes occurring in real materials. One of such processes is the segregation/depletion of vacancies or Cr atoms at grain boundaries (GBs). In this contribution the density functional theory (DFT) and molecular dynamics (MD) results of vacancies and Cr atoms stability at the Fe Σ5(210) GB are presented. Using MD quenching at zero temperature we investigate possible structural modifications of this GB. We found different configurations of the GB and their energies. For these purposes, the state-of-the-art interatomic potentials were utilized. Configurations from MD were then relaxed by means of the DFT to confirm their stability. The most stable one was employed to investigate the Cr atoms and vacancies at the GB under consideration in order to have a first idea which sites attract or repel Cr atoms and vacancies.

MM 30.3 Wed 10:45 H4

Computational study of the intergranular fracture strength of transition metals in the presence of impurity atoms — •Arshad Tahir, Venkata Naga Sudheer Ganisetti, Rebecca

Janisch, and Alexander Hartmaier — ICAMS, Ruhr University Bochum, Germany

Grain boundaries play an important role during plastic deformation and failure of poly-crystals. In case of the refractory metals e.g. molybdenum and tungsten which are the materials of interest in high-temperature applications, the reduction of strength due to grain boundary embrittlement is especially large. The presence of defects e.g. point defects at the grain boundaries affect their mechanical properties, which in turn alter the hardness or fracture toughness of poly-crystals favorably or adversely. Carbon as a point defect has been reported to increase the strength of bcc metals whereas hydrogen and oxygen are assumed to be detrimental for grain boundary strength. In order to investigate the strengthening and em-brittling nature of above mentioned impurity atoms at grain boundaries, a systematic study of a Σ 5 (310)[001] symmetrical tilt grain boundary (Σ5 STGB) in molybdenum, tungsten and iron has been carried out. Atomistic scale uni-axial mechanical tests with loads perpendicular to the grain boundary were performed for all the afore mentioned systems using ab-initio density functional theory calculations. From these results, traction separation data has been derived that is being used for the parameterization of cohesive zone model to predict the inter-granular fracture at continuum level using finite element analysis.

MM 30.4 Wed 11:00 H4

A Finite Element Analysis of the Fracture Behavior of Tungsten at the micro scale — •Christoph Bohnert[1,2], Nicola Julia Schmitt[2], Sabine Maria Weygand[1], and Oliver Kraft[2] — [1]Karlsruhe University of Applied Sciences, Department of Mechanical Engineering and Mechatronics, D-76133 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), D-76344 Eggenstein-Leopoldshafen, Germany

Due to its high melting point tungsten has the potential to be used as a structural material in future energy applications. However, one of the challenges is to deal with the brittleness at room temperature, where the fracture behavior of polycrystalline tungsten is strongly influenced by the grain structure and texture as well as sample dimensions. The aim of the present work is to numerically analyze crack initiation and growth in single crystal tungsten microbeams and to relate it to corresponding experimental observations.

A finite element model was developed to study the fracture behavior of the cantilever at different crack orientations. As plastic deformation is observed at the crack tip, plastic deformation is implemented using a crystal plasticity approach which allows for specifying the crystal orientation. Crack initiation and growth are treated by using the cohesive zone method. Based on experimental oberservations, the material parameters are estimated, and the fracture model has been applied to simulate microbending tests. The simulations allow for comparison of the computed with the measured load displacement curves as well as details of the fracture process, ultimately at various length scales.

MM 30.5 Wed 11:15 H4

A high-resolution look at crack tip deformation — •Christoph Kords[1], Philip Eisenlohr[1], Arshad Tahir[2], Rebecca Janisch[2], and Franz Roters[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

The deformation behavior around a pre-existing intergranular crack is simulated in a two-dimensional setting for a grain boundary in bcc Mo. The associated boundary value problem is solved at very high spatial resolution (millions of pixels) by means of a recently implemented spectral method based on fast Fourier transforms. The cohesive properties of the grain boundary are derived from ab-inito density functional theory calculations. Our interest focuses on the conditions under which the theoretical interface strength obtained from such atomistic calculations will be locally reached in the mesoscale simulation when dislocation-mediated crack tip plasticity is included. In this study we will investigate the influence of spatial resolution on the one hand and of the physical rigorousness of the crystal plasticity description on the other hand. To the latter end, three different crystal plasticity models are to be compared: a frequently employed (standard) power-law dislocation kinetics coupled with a phenomenological hardening description; a dislocation mechanics-based description considering dislocation densities and their reactions; and finally the same (second) model but with additional integration of the dislocation transport that is always associated with plasticity.

MM 31: Computational Materials Modelling - Diffusion & Kinetics II

Time: Wednesday 10:15–11:30 Location: H24

MM 31.1 Wed 10:15 H24

AKMC simulations of solid-solid phase transformations in molybdenum — •Ari Harjunmaa, Jutta Rogal, and Ralf Drautz — ICAMS – Ruhr University Bochum, 44789 Bochum, Germany

Molybdenum is a refractory metal used as an alloying element to improve the properties of high-performance materials such as Ni-base superalloys. A common problem in these materials is the formation of topologically close-packed (TCP) phases, which deprive the bulk matrix of the alloying elements and cause the material to become brittle. It is therefore of utmost importance to understand the atomistic processes at work in solid-solid phase transitions leading to the formation of TCP phases. We begin this task by investigating interfaces between the TCP A15 and the cubic BCC phases in molybdenum. We use adaptive kinetic Monte Carlo simulations to discover atomistic processes at the interfaces and to model the time evolution of the systems in question. We also investigate the energetics and stability of the interface structures, and we evaluate the reliability of the employed interatomic potentials by comparing results obtained from density functional theory to those from bond-order and empirical potential simulations.

MM 31.2 Wed 10:30 H24

A first-principles study of energetics of As, Sb and Bi along selected deformation paths and its application to structure of epitaxial thin films — •Martin Zouhar[1] and Mojmír Šob[1,2,3] — [1]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We present a comprehensive density-functional-theory study of total energy and structural properties of As, Sb and Bi in their A7 ground state and three cubic modifications. All the structures studied are newly described on equal footing with the help of a hexagonal unit cell and can be represented as points in a 3-dimensional parameter space spanned by atomic volume, trigonal distortion and an internal parameter u of the A7 structure (for cubic structures, u=0.25). We calculated the total energies along selected deformation paths by pseudopotential VASP code, displayed them in contour plots as functions of the above-mentioned parameters, identified energy extrema corresponding to the four basic structures and found minimum energy paths connecting selected structures. The calculated energy profiles are employed to determine the structure parameters of As, Sb and Bi thin films on various substrates with the (111) cubic or (0001) hexagonal geometry. Overall good agreement with available experimental data has been found, but we also provide many theoretical predictions which may motivate experimentalists for a deeper study of these systems.

MM 31.3 Wed 10:45 H24

Phase-field modeling of anisotropically diffusional growth during solid solid transformation: Li-insertion in $LiFePO_4$-cathods for rechargeable Li-ion battery applications — •Holger Federmann, Michael Fleck, and Heike Emmerich — Material and Process Simulation, University of Bayreuth, Germany

The delithiation process in $LiFePO_4$ is considered to be a first-order transformation process, where a Li-rich phase transforms into an Li-depleted one. In order to shed light on the delithiation process in $LiFePO_4$-cathodes, a continuum phase field model was developed to describe the dynamics of Li-intercalation there. The cathode consists of nanoscale olivine particles and the model describes the phase transformation through Li-insertion. Within the phase-field method, moving phase boundaries between different phases are treated as diffuse interfaces of finite width. Then, the evolution of the diffuse phase boundary

is driven by the mechanics and the thermodynamics of the adjacent bulk phases. In turn, the motion of the diffuse interface strongly influences the bulk properties such as mechanical or thermodynamical degrees of freedom. Generally, such a diffuse interface approach provides an elegant way to incorporate the complicated effects that occur in these materials, such as the highly anisotropic ionic mobility of the Li-ions in the olivine bulk crystal, the electrochemical reactions at the phase boundary, stress and strain effects due to density differences between the phases. Finally, this model at hand, it could be shown that the interpolation on level of eigenstrains should be preferred for the calculation of the elastic free energy densities of the system.

MM 31.4 Wed 11:00 H24

Defect-domain wall interactions in ferroelectric materials — •Anand Chandrasekaran[1,2], Dragan Damjanovic[2], Nava Setter[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Ceramics Laboratory, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Hardening and softening of ferroelectric materials can be engineered through the addition of dopants, and is a key technique to tailor dielectric and piezoelectric properties. Hardening is typically driven by the addition of acceptor dopants, and leads to small electromechanical coefficients and pinched hysteresis loops. Softening can be induced by the addition of donor dopants, which leads to large electromechanical coefficients and open hysteresis loops. Doping results in the formation of defects which interact with the domain walls present in the material. We use here first-principles calculations to show how acceptor dopants lead to the formation of defect complexes which align with the polarization axis and stabilize the ferroelectric domains. We corroborate the AC and DC conductivity data obtained in acceptor-doped materials with first-principles activation energies for the hopping of oxygen vacancies, obtained through nudged elastic-band calculations (NEB). We also calculate the NEB barrier energies for the movement of domain walls in the presence of various defects. As a result, we show how defects and defect associates can influence the mobility of domain walls leading to hardening or softening.

MM 31.5 Wed 11:15 H24

First-principles thermodynamics of paramagnetic fcc iron — •Fritz Körmann, Blazej Grabowski, Biswanath Dutta, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

A key issue of thermodynamic first-principles modeling of paramagnetic materials is the interplay of magnetic and atomic degrees of freedom. Practical approaches allowing the computation of atomic forces at finite magnetic temperatures are up to now only rarely available, but are decisive for an accurate description of the thermodynamics in many material systems. For example, first-principles predictions for paramagnetic iron are typically based on empirical approximations, e.g., the 2-states spin model. For this reason, we have recently developed an ab initio approach to obtain effective paramagnetic atomic forces [1]. They are obtained from SQS structures for the magnetic disorder combined with a spin-space averaging procedure. Employing this method we calculate the paramagnetic quasi-harmonic (vibrational) free energy for fcc iron. Adding electronic and magnetic contributions we obtain the complete free energy surface. The derived thermodynamic properties such as phonon spectrum, expansion coefficient, and bulk modulus are in good agreement with experiment.

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B 85, 125104 (2012).

MM 32: Topical Session: TEM-Symposium - Structure-Property / In-Situ I

Time: Wednesday 10:15–11:30 Location: H25

Topical Talk MM 32.1 Wed 10:15 H25

Structure and deformation processes of nanocrystalline metals characterized by ACOM-STEM in combination with in-situ straining — Aaron Kobler[1,2], Horst Hahn[1,2], and •Christian Kübel[1,3] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, 76021 Karlsruhe, Germany — [2]Technische Universität Darmstadt (TUD), KIT-TUD Joint Research Laboratory Nanomaterials, 64287 Darmstadt, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe Nano Micro Facility, 76021 Karlsruhe, Germany

Understanding the deformation mechanisms in nanocrystalline (nc) metals and alloys is crucial for improving their performance and stability as needed for technical applications. In-situ deformation studies using XRD have contributed significantly to our current understanding of nc metals. However, it is difficult to understand the local processes and thin-film properties based on bulk measurements. These local processes are traditionally investigated using classical BF/DF-TEM. As an alternative, automated crystal orientation mapping (ACOM) inside a TEM has recently been developed for nanocrystalline materials as it allows identification of the crystallographic orientation of all crystallites and detects the CSL special boundaries within the imaged area. We have implemented ACOM on a FEI Tecnai F20 in micro-probe (up) STEM mode, that allows us to also acquire (fast) STEM reference images. We combined this ACOM-STEM imaging with in-situ straining inside the TEM using Hysitron*s Picoindenter. First investigations were conducted on magnetron sputtered Au samples and deformation of these films inside the TEM allowed us to follow the process of grain growth, grain rotation and (de)twinning in nc Au with increasing strain. New results will discuss the influence of alloying content in PdxAu1-x on the deformation behavior.

MM 32.2 Wed 10:45 H25

Grain size reduction by heating in nanocrystalline FeAl - a mystery solved by TEM — Christoph Gammer, Clemens Mangler, •Hans-Peter Karnthaler, and Christian Rentenberger — Universität Wien, Physik Nanostrukturierter Materialien, Boltzmanngasse 5, 1090 Wien, Austria

Bulk nanocrystalline materials show improved mechanical properties as compared to their coarse grained counterparts. Due to the high density of grain boundaries a thermodynamic driving force for grain growth exists and therefore, the thermal stability of a nanograined structure is usually low. In contrast, we show that in the present case of intermetallic FeAl made nanocrystalline by severe plastic deformation, a reduction of the grain size is occurring by heating connected with an increase in hardness [1]. High pressure torsion deformation of B2 ordered FeAl leads to a nanocrystalline material with strongly reduced long-range order. The samples show nanosized grains (about 70nm) with a high defect density and highly irregular grain boundaries. In-situ and post mortem TEM of thermally treated samples reveal a recurrence of the B2 superstructure [2], the re-arrangement of dislocations and what is rather unexpected, a reduction in grain size by a factor of 2. It is proposed that the decrease of the grain size during heating is linked to the recurrence of the long-range order by the interaction of the dislocations with the growing ordered domains. Therefore, subgrain boundaries turn into grain boundaries at a temperature too low for grain growth. [1] C. Mangler et al. Acta Mater 58 (2010) 5631. [2] C. Gammer et al. Scripta Mater 65 (2011) 57.

MM 32.3 Wed 11:00 H25

Combined use of ex-situ and in-situ TEM for the analysis of the nanocrystallization of bulk amorphous NiTi — •Martin Peterlechner[1], Thomas Waitz[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, WWU Münster, Germany — [2]Physics of Nanostructured Materials, University of Vienna, Austria

A NiTi shape memory alloy was subjected to severe plastic deformation by repeated cold rolling (RCR). RCR yields almost complete amorphization. A small volume fraction of nanocrystalline debris is embedded heterogeneously in the amorphous matrix. Upon annealing nanocrystallization occurs. The crystallization kinetics were analyzed using ex-situ and in-situ transmission electron microscopy (TEM) experiments. Ex-situ TEM investigations were carried out of bulk samples crystallized at 307°C (270 min) in a calorimeter that allows precise control of the temperature. Ex-situ TEM specimens were analyzed at room temperature. Additional, in-situ TEM heating was carried out at a nominal temperature of 307°C. From in-situ TEM it can be concluded that hard-impingement is present. Therefore, the grain sizes formed by ex-situ nanocrystallization can be used to analyze the ki-

netics based on hard impingement models. The crystallization causes grains with a bimodal size distribution. This is explained considering the heterogeneous distribution of nanocrystals left in the amorphous matrix that can act as nucleation sites of new grains. Since the number density of the nanocrystalline debris depends on the degree of deformation, both the degree of the deformation and the crystallization temperature can be used to tailor the grain size.

MM 32.4 Wed 11:15 H25

TEM study of Co_3Ti made amorphous by high pressure torsion — •David Geist, Christoph Gammer, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, 1090 Vienna, Austria

Amorphous structures can be achieved by a solid state transformation of the crystalline structure using severe plastic deformation. This has been successfully achieved by applying high pressure torsion (HPT) deformation in the case of $L1_2$ ordered intermetallic Zr_3Al [1,2]. In the present work the evolution, structure and stability of the amorphous state of bulk Co_3Ti were studied on multiple length scales using a combination of scanning (SEM) and high resolution transmission electron microscopy (HRTEM) methods. $L1_2$ ordered Co-23at.%Ti samples were deformed by HPT to different degrees of deformation. The SEM investigations using back scattered electrons reveal that the material shows a tendency to amorphization localized in the form of bands. The TEM results of the amorphous regions show that a high density of nanosized crystals having a crystalline structure different from the initial material is embedded in the amorphous phase. Electron diffraction and HRTEM reveal the presence of nanocrystals with Co_2Ti structure showing a modified stacking sequence. Their structure is compared to that resulting from devitrification of the amorphous regions during thermal treatment. [1] D. Geist, C. Rentenberger, H. P. Karnthaler. Acta Mater. **59** (2011) 4578. [2] D. Geist, S. Ii, K. Tsuchiya, H.P. Karnthaler, G. Stefanov, C. Rentenberger. JAllComp **509** (2011) 1815.

MM 33: Structural Materials

Time: Wednesday 10:15–11:30 Location: H26

MM 33.1 Wed 10:15 H26

Identifying isotropic auxetic modes in planar crystallographic frameworks — •Holger Mitschke[1], Gerd E. Schröder-Turk[1], Klaus Mecke[1], Patrick W. Fowler[2], and Simon D. Guest[3] — [1]Theoretische Physik, Univ. Erlangen — [2]Depart. Chemistry, Univ. Sheffield, UK — [3]Depart. Engineering, Univ. Cambridge, UK

Auxetic materials, i.e. with a negative Poisson's ratio, possess typical microstructures enabling deformations with either rotating or reentrant elements. Here we idealise planar auxetic microstructures by frameworks of j joints connected by b rigid bars and restrict our study to frameworks with crystallographic symmetry. An observation is that known auxetic microstructures map to non-rigid (floppy) frameworks [1]. Under this assumption an analysis of the types of mechanisms w.r.t. auxeticity seems a promising approach to identify and understand auxetic materials in a simplified but often sufficient manner. The two-dimensional Calladine-Maxwell counting rule $m - s = 2j - b + 3$ gives the net mobility where m is the number of mechanisms and s the number of self-stresses. This rule can be extended by taking crystallographic symmetries into account [2] and has recently been extended to allow for periodicity [3]. In this talk the application to planar *hexagonal* and *square* groups is presented which gives sufficient counts of the number of symmetry-detectable isotropic auxetic mechanisms.
[1] Mitschke H. et.al. (2013), Proc. R. Soc. A, 469.
[2] Fowler, P.W. and Guest, S.D. (2000), Int. J. Solids. Struct, 37.
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MM 33.2 Wed 10:30 H26

Atom Probe Tomography of Aluminum Lithium Based Alloy — •Muna Khushaim[1], Judith Leese[2], Torben Boll[1], Ferdinand Haider[2], and Talaat Al-Kassab[1] — [1]King Abdullah University of Science and Technology (KAUST), Division of Physical Sciences and Engineering, Thuwal 23955-6900. Saudi Arabia — [2]University of Augsburg, Inst. f. Physik, D-86159 Augsburg, Germany

Aluminum alloys exhibiting an improved weight/toughness ratio have been the primary materials for some structural components of aircraft applications. Such alloys can be strengthened through an imposed precipitation by a thermo-mechanical aging treatment. The primary strengthening precipitates $T_1(Al_2CuLi)$ and other metastable phases such as $\theta'(Al_2Cu)$ and $\delta'(Al_3Li)$ are expected to form at different stages of the post heat treatment of the alloy. Hence, an understanding of the distribution of alloying elements and of prestages of precipitation becomes imperative to understand the link between the microstructure and mechanical functionality of the respective alloy. In this study the Laser Assisted Wide Angle Atom Probe Tomography (LAWATAP) was applied to investigate the decomposed microstructure and the possible origins of hardening precipitates in a commercial Al-Li-Cu alloy (AA2195).

MM 33.3 Wed 10:45 H26

Characterization of the microstructure in Mg based alloy — •Arwa Kutbee[1], Talaat Al-Kassab[1], Xinhua Zhu[2], Zhiguo Liu[3], and Wenzheng Zhang[4] — [1]King Abdullah University of Science & Technology, Division of Physical Sciences and Engineering, Thuwal, 23955-6900, Kingdom of Saudi Arabia — [2]National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China — [3]National Laboratory of Solid State Microstructures, Department of Materials Science and Engineering, Nanjing University, Nanjing 210093, China — [4]Laboratory of Advanced Materials, Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Magnesium based alloys are prospective materials for light weight application. Their creep and mechanical properties can be largely modified by precipitation hardening. In this paper, we report on the decomposition behavior of Mg-6.5Sn-3.3Zn-0.2Mn wt.% alloy using transmission electron microscopy (TEM) and Atom Probe Tomography (APT). Two techniques for TEM sample preparation have been employed: Focused ion beam (FIB) and ion beam milling. TEM lamella prepared by FIB at certain energy of the ion source might largely influence the crystalline structure in these alloys. Whereas, the ion beam milling method provided a preferable route to prepare transparent specimen for microstructural characterization. The TEM micrographs showed a lath shaped precipitates in the Mg matrix. APT composition analysis of the decomposed microstructure will be also presented and discussed.

MM 33.4 Wed 11:00 H26

Study of the phase transformation in SiC/AlN ceramic composite — •Naeem-Ur-Rehman Minhas[1], Jianye Wang[2], Finn Giuliani[2], Luc Vandeperre[2], and Talaat Al-Kassab[1] — [1]Physical Sciences and Engineering Division, King Abdullah University of Science & Technology, 4700, Thuwal, 23955-6900, Saudi Arabia — [2]Centre for Advanced Structural Ceramics, Department of Materials, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

Silicon carbide (SiC) is used in various high temperature applications for its high hardness. However, the hardness of SiC drops with temperature because thermal activation of dislocations allows them to overcome the lattice resistance. Hence to enhance the high temperature properties of silicon carbide other strengthening mechanisms are needed. A tentative phase diagram of silicon carbide and aluminium nitride (AlN) points towards a region where perhaps decomposition occurs. Such phase separation should strengthen the resistance to dislocation glide or creep of SiC. The first aim is to produce a solid solution of SiC and AlN, and this will be followed by a heat treatment to induce the phase separation. X-ray diffraction results show the formation of a single phase with a simple hexagonal crystal structure confirming the formation of a solid solution. The decomposition path of the as prepared material as investigated with x-ray diffraction and transmission electron microscopy and Atom Probe Tomography will be presented and discussed within this contribution.

MM 33.5 Wed 11:15 H26

Stability of TCP phases in Co-based superalloys: Comparison of ab initio results with structure maps — •Jörg Kossmann, Thomas Hammerschmidt, and Ralf Drautz — ICAMS,

Ruhr-Universität Bochum, Germany

Single crystal superalloys based on Ni are commonly used as turbine blades in industrial gas turbines for aero-engines and power plants. The observation of a stable $Co_3(Al,W)$ phase with $L1_2$ structure showed that single crystal alloys based on Co can also be fabricated. Such Co-based systems exhibit similar hardening mechanisms at a potentially higher melting point. Hence, we compare Co-based systems using high-throughput density functional theory calculations. In particular, we determine the heat of formation of the A15, C14, C15, C36, μ, χ and σ phases (with every possible stoichiometry) of the binary systems Co-W, Al-W, and Co-Al. We show that our DFT results are in line with a recently derived structure map based on experimental data. This work is part of the collaborative research center SFB/TR 103.

MM 34: Topical Session: Fundamentals of Fracture - Fracture at the Atomistic Scale

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

MM 34.1 Wed 11:45 H4

Intergranular vacancies impact fracture — •Döme Tanguy — Université de Lyon 1 France

Hydrogen has a strong binding to vacancies, which could lead to large vacancy concentrations. We study, by atomistic simulations, their possible impact on grain boundary fracture. Intergranular vacancy clusters are generated by Monte Carlo. The configurations are passed to MD and the critical loads for dislocation emission are compared to those for crack propagation. We report the minimum void size that triggers brittle propagation by "nano void" growth and discuss the crossover from intrinsic ductility to brittleness.

MM 34.2 Wed 12:00 H4

hydrogen enhanced dislocation emission at a crack tip — •yu wang[1,2], damien connétable[2], and döme tanguy[1] — [1]Laboratoire de Physique de la Matière Condensée et Nanostructures, Université Claude Bernard Lyon 1, 43 Boulevard du 11 Novembre 1918, F 69622 Villeurbanne, France — [2]CIRIMAT, CNRS-UPS-INPT, ENSIACET 4 allée Emile Monso, BP 44362, F 31030 Toulouse, France

The influence of hydrogen on plasticity is an essential component of the modelling of H induced damage in structural metallic alloys. In this work, we study an idealized configuration where an atomistically sharp crack is loaded in mixed mode until a straight dislocation is emitted directly at the tip. It is shown, by Molecular Statics calculations using empirical EAM potentials, that the model proposed by Rice, which relates the critical stress intensity factor for emission (Ke) to the unstable staking fault energy (γus), is exact for dislocations moving along the crack plane (modes II or III dominate mode I), provided the influence of the mode I is taken into account in the γus calculation. The interest of combining Molecular Statics with the Rice model is that γus can be calculated on a system simple enough to be handled by ab initio methods. When dealing with hydrogen, on the contrary, there is no a priori knowledge how to introduce the H induced relaxations in the γus calculation, still preserving the relation between by γus and ke established by Rice. Therefore, Molecular Statics calculations with an empirical EAM potential for Al-H and Ni-H, on a large simulation box containing a crack, γus calculations with EAM potentials and ab initio calculations should be performed in parallel.

MM 34.3 Wed 12:15 H4

Multiscale Modelling of Hydrogen Embrittlement in Zirconium Alloys — •Jassel Majevadia[1], Mark Wenman[1], Daniel Balint[1], Adrian Sutton[1], and Roman Nazarov[2] — [1]Imperial College London, UK — [2]MPIE, Dusseldorf, Germany

Delayed Hydride Cracking (DHC) is a commonly occurring embrittlement phenomenon in zirconium alloy fuel cladding within Pressurized Water Reactors (PWRs). DHC is caused by the accumulation of hydrogen atoms taken up by the metal, and the formation of brittle hydrides in the vicinity of crack tips. The rate of crack growth is limited by the rate of hydrogen diffusion to the crack, which can be modelled by solving a stress driven diffusion equation that incorporates the elastic interaction between defects. This of interest in the present work.

The elastic interaction is calculated by combining defect forces determined through Density Functional Theory (DFT) simulations, and an exact solution for the anisotropic elastic field of an edge dislocation in Zr. making it possible to determine the interaction energy without the need to simulate directly a hydrogen atom in the presence of a crack or dislocation, which is computationally prohibitive with DFT.

The result of the elastic interaction energy calculations can be utilised to determine the segregation of hydrogen to a crack tip for varying crack tip geometries, and in the presence of other crystal defects. This is done by implementing a diffusion equation for hydrogen within a discrete dislocation dynamics simulation. In the present work a model has been developed to demonstrate the effect of a single dislocation on hydrogen diffusion to create a Cottrell atmosphere.

MM 34.4 Wed 12:30 H4

Multiscale Simulation of Brittle Fracture in Oxides and Semiconductors — •James Kermode — King's College London, Physics Department, London, WC2R 2LS, United Kingdom

Fracture is probably the most challenging 'multi-scale' problem: crack propagation is driven by the concentration of a long-range stress field at an atomically sharp crack tip. This creates a complex dynamical system with strongly coupled length scales. An accurate description of the chemical processes occurring in the small crack tip region is therefore essential, as is the inclusion of a much larger region in the model systems. Both these requirements can be met by combining a quantum mechanical (at the DFT level) description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) technique such as the 'Learn on the Fly' (LOTF) scheme. Here, we consider silicon and silica as prototypical semiconductor and oxide materials, respectively. The elastic and thermodynamic behaviour of silicon can be accurately described with simple interatomic potentials, while for silica a polarizable force field is required. Examples of the application of these techniques to fracture problems include low-speed dynamical fracture instabilities in silicon, interactions between moving cracks and material defects such as dislocations or impurities, very slow crack propagation via kink formation and migration, and chemically activated fracture, where cracks advance under the concerted action of stress and corrosion by chemical species such as oxygen or water.

MM 34.5 Wed 12:45 H4

Brittle fracture of rutile TiO_2: a first principles study — •Beatrix Elsner, Wolfgang Heckel, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

The potentiality of catastrophic failure poses a major challenge for the engineering application of brittle materials such as ceramics. Hence a fundamental understanding of the atomistic processes involved in brittle fracture is essential. Using density functional theory we have studied the failure of rutile titanium dioxide (TiO_2) in loading mode I accounting for various cleavage plane orientations. For ideal brittle cleavage no surface relaxations are allowed and the universal binding energy relation (UBER) [1] can be applied to calculate the theoretical cleavage energy and corresponding strength. This yields the (110) and (100) planes as the equally most likely cleavage planes. Further, structural relaxations have been treated as they have a significant influence on the cleavage properties by lowering the cleavage energy. Unlike for metals [2] the onset of cleavage in TiO_2 cannot be easily derived from the energy separation curves and the relation between elasticity and cleavage will be discussed.

Supported by DFG, SFB 986, project B3.

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[2] P. Lazar, R. Podloucky, *Phys. Rev. B* **78**, 104114 (2008).

MM 35: Computational Materials Modelling - Phonons & Phase Stability

Time: Wednesday 11:45–13:00 Location: H24

MM 35.1 Wed 11:45 H24

Phonon dispersions in iron: comparing empirical potentials with first-principles calculations and experimental results — •Daniele Dragoni[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Consiglio Nazionale delle Ricerche, Milano, Italy

Many empirical potentials for iron and its alloys are available in literature. Their performance and reliability has been tested for energetics, thermodynamic properties, and relative bcc-fcc stability under martensitic transformation (Bain path). We focus here on phonon dispersions as a robust indicator of potentials' quality. Both the low temperature bcc phase (ferromagnetic α-phase up to 1043 K, and paramagnetic β-phase up to 1184 K) and the higher temperature fcc paramagnetic γ-phase (between 1184 K and 1670 K) are considered and compared to experimental results and, where available, to ab-initio data. This approach provides valuable insight about the relative accuracy of potentials in treating long- and short-wavelength vibrations and elastic constants at different temperatures and for distinct solid phases.

MM 35.2 Wed 12:00 H24

Ab initio finite temperature description of α Ti including anharmonic contributions — •Dominique Korbmacher, Albert Glensk, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti and its alloys are technologically relevant for instance for aircraft or medical applications. *Ab initio* methods based on density-functional theory (DFT) are now routinely used to investigate T=0 K properties such as, e.g., the influence of alloying elements on titanium's mechanical properties. In contrast, finite temperature DFT studies are rare and, in particular, limited to approximations such as the quasiharmonic model. While the latter is an accurate approximation for many elements, deviations of $\approx 15\%$ are found for the heat capacity of α Ti (hcp) at higher temperatures [1].

In the present study, we investigate the influence of anharmonic excitations on the thermodynamics of α Ti. To overcome long CPU times we use here the recently developed UP-TILD method [2], a coarse graining scheme allowing to reduce the computation time significantly while keeping high accuracy. In the talk we present the contribution of anharmonicity to various thermodynamic quantities of α Ti and discuss its balance with respect to the other finite temperature excitations. Finally, we reveal whether it can account for the observed discrepancy with experiment or whether the problem originates from an inherent shortcoming of the employed DFT functionals.

[1] Z. G. Mei et al., PRB **80**, 104116 (2009).
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MM 35.3 Wed 12:15 H24

Modelling phonons in Si_xGe_{1-x} alloys — •Ankita Katre, Georg K. H. Madsen, and Ralf Drautz — ICAMS,Ruhr-Universität Bochum, 44780 Bochum, Germany

Si_xGe_{1-x} alloys are important materials both for the electronics industry[1] and for thermoelectric applications at high temperature[2]. Several experimental and theoretical studies report the enhancement of dimensionless figure of merit (zT) of Si_xGe_{1-x} random alloys by reducing thermal conductivity[3,4]. The phonon calculations required to determine the thermal conductivity of random alloys are computationally expensive using DFT. We have therefore developed a model for obtaining phonon spectra of Si_xGe_{1-x} random alloys. The model parameters are extracted from DFT-calculated force constant matrices for pure Si and pure Ge. We include the contributions upto second nearest neighbour as we find that the phonon frequencies obtained by considering only the onsite and first nearest neighbour force constant matrices are not sufficient for approximating the acoustic phonon modes. The model allows us to determine the phonon frequencies for Si_xGe_{1-x} alloys accurately and efficiently without performing *ab initio* calculations.

[1] J. Ouellette, The Industrial Physicist 8, 22 (2002).
[2] G. A. Slack and M. A. Hussain, J. Appl. Phys. 70, 2694 (1991).
[3] H. Lee, D. Vashaee, D. Z. Wang, M. S. Dresselhaus, Z. F. Ren, and G. Chen, J. Appl. Phys. 107, 094308 (2010).
[4] C. Bera, N. Mingo, and S. Volz, Phys. Rev. Lett. 104, 115502 (2010).

MM 35.4 Wed 12:30 H24

Comparison of phonon frequencies and polarization vectors obtained from fitted force constants or from ab initio force constants — •Christian Illg[1], Bernd Meyer[2], and Manfred Fähnle[1] — [1]Max-Planck-Institut für Intelligente Systeme, 70569 Stuttgart, Germany — [2]Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg, 91052 Erlangen, Germany

The calculation of electron-phonon scattering matrix elements is necessary in many physical contexts and requires reliable information about phonon frequencies and polarization vectors. One can calculate the phonon frequencies and polarization vectors from the dynamical matrix which is the Fourier-transformed force-constant matrix. The force constants can either be determined by a fit to experimental data or by an ab initio calculation. It is well known that the fitted force constants cannot be determined unambiguously since the polarization vectors are hard to measure and do not enter the fit [1]. A unitary transformation would alter the force constants while leaving the frequencies unchanged (but the polarization vectors would change). We compare the frequencies and polarization vectors in the whole Brillouin zone obtained from fitted force constants and obtained from ab initio force constants [2]. The results are important to make a statement on the reliability of phonon polarization vectors obtained from fitted force constants.

[1] R. S. Leigh, B. Szigeti, V. K. Tewary, Proc. R. Soc. London, Ser. A 320, 505 (1971)
[2] C. Illg, B. Meyer, M. Fähnle, Phys. Rev. B 86, 174309 (2012)

MM 35.5 Wed 12:45 H24

Atomistic Modelling of Flexoelectricity in Periclase — Philipp Beck, •Johannes Roth, and Hans-Rainer Trebin — ITAP, Universität Stuttgart

We present a molecular dynamics study of flexoelectricity in periclase. Applying a polarizable effective interaction force field, collective flexoelectric response of an inhomogeneously strained periclase sample can be visualized for the first time. The linear response in periclase is verified by simulations. Two of the linear coupling coefficients can be determined as well as the flexoelectric free energy density as a function of strain gradient. We present a first time modelling of flexoelectric domain building. It turns out that domains in periclase are well separated by a wall of Néel-type.

MM 36: Topical Session: TEM-Symposium - Structure-Property / In-Situ II

Time: Wednesday 11:45–13:00 Location: H25

MM 36.1 Wed 11:45 H25

A novel technique for measuring density changes in shear bands of metallic glasses — •Harald Rösner[1], Christian Kübel[2,3], Martin Peterlechner[1], Joachim Bokeloh[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), — [3]Karlsruhe Nano Mircro Facility, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

The deformation process in glasses is different from that in crystalline materials because there is no crystal lattice and consequently no defects such as dislocations, twins or grain boundaries are available as deformation carriers for an easy flow mechanism. Deformation tests on glasses have shown that when the applied load exceeds the elastic range the plastic flow is confined to narrow regions called shear bands. In TEM, shear bands are distinguished from the surrounding

amorphous matrix as regions of lower contrast, which is thought to be associated with an increase in free volume and thus a lower density. We describe here a new approach to measure density changes between the amorphous matrix and the shear bands of metallic glasses using the information from electron-energy loss spectra (EELS) and the high-angle annular dark-field scanning transmission electron (HAADF-STEM) signal. We found for melt-spun Al88Y7Fe5 ribbons, surprisingly, an enormous decrease in density in the sheared zones of 6.7%, which we associate with the free volume in the shear bands.

MM 36.2 Wed 12:00 H25

Ordering in deformed bulk metallic glasses studied by TEM — Christoph Gammer[1], Denise Beitelschmidt[2], Simon Pauly[2], David Geist[1], Jürgen Eckert[2], Hans-Peter Karnthaler[1], and •Christian Rentenberger[1] — [1]Universität Wien, Physik Nanostrukturierter Materialien, Boltzmanngasse 5, 1090 Wien, Austria — [2]IFW Dresden, Institut für Komplexe Materialien, Helmholtzstraße 20, 01069 Dresden, Germany

Bulk metallic glasses are characterized by an amorphic atomic arrangement, still it is assumed that some medium range order (MRO) is present. This contributes to many outstanding properties as high strength, high elastic limits and in special cases combined with some plasticity. Despite intense research activities, the details of the structure are generally not well understood. Here we use transmission electron microscopy (TEM) methods to study the structure of an bulk metallic CuZrAlAg glass. The medium range order of the amorphous structure is unravelled experimentally using fluctuation electron microscopy that measures statistical fluctuations in the scattering of electrons as a function of spatial frequencies [1]. Based on this coarse graining TEM method the intensity fluctuations in dark-field images indicate the presence of B2 like medium range order. The differences in the MRO of as cast and deformed bulk metallic CuZrAlAg glass are investigated.

[1] M.M.J. Treacy and J.M. Gibson, Acta Cryst. 52 (1996) 212.

MM 36.3 Wed 12:15 H25

In situ TEM deformation of Au nanowires — •Burkhard Roos[1], Bahne Kapelle[1], Torben Erichsen[1], Gunther Richter[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart

Increasing strength with decreasing size is a common phenomenon in metals, and is often explained in terms of dislocation pile-ups and interactions. However, for free standing samples with dimensions below 150 nm, dislocation storage is hard to envision and a convincing explanation for the high strength is still 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 250 nm have been used for this study. Stacking faults appear during tensile deformation as a result of the nucleation and motion of partial dislocations. The stacking faults form homogenously along the wire length on {111} planes. The stacking faults thicken into nanotwins through the sequential activation of partial dislocations on neighbouring (111) planes. Post-deformation TEM studies show that fracture occurs at a nanotwin. In contrast bending of identical wires leads to the nucleation of full dislocations. A quantitative model based on classical nucleation theory will be presented which explains the observed difference in deformation mode. Implications for different materials and loading geometries will be discussed.

Topical Talk MM 36.4 Wed 12:30 H25

In-situ transmission electron microscopy — •Henny Zandbergen — Kavli Institute of Nanoscience, TUDelft, Delft, The Netherlands

After a decade of great improvements in the optical performances of high-resolution electron microscopes, the developments in the next decade of transmission electron microscopy (TEM) will be mainly in the development of in-situ electron microscopy and 3D analysis on the atomic level. In Delft we have focused on in-situ (TEM), using in part MEMS (micro electro mechanical systems) devices to overcome size related problems due to the limited available space in the TEM for sample manipulation. In Delft we are using routinely MEMS based holders for heating, for applying electrical currents and heating under a gas atmosphere.

In the talk in-situ TEM examples will be given of electromigration in metal nanobridges, (de)hydrogenation of hydrogen storage materials, changes in the shapes and crystal structures of semiconductor nanoparticles and the sculpting of grapheme into nanoribbons.

MM 37: Mechanical Properties I

Time: Wednesday 11:45–13:00 Location: H26

MM 37.1 Wed 11:45 H26

γ' Hardened Cobalt-Base Superalloys - A New Class of High Temperature Materials — •Steffen Neumeier, Christopher Zenk, Alexander Bauer, and Mathias Göken — Lehrstuhl Allgemeine Werkstoffeigenschaften, Department Werkstoffwissenschaften, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland

Conventional Co-based alloys are suitable materials for use in corrosive environments at high temperatures. However, the classic Co-based alloys with high Chromium contents cannot compete with γ' (Ni3Al) hardened Ni-base superalloys in terms of strength as they are only carbide and solid solution hardened. Accordingly, these alloys are only used as materials for static parts in gas turbines for energy conversion, for example. However, this situation could change in the future due to the discovery of the ternary compound Co3(Al,W) in 2006. This stable intermetallic phase with L12 crystal structure is in equilibrium with the face centered cubic Co solid solution and therefore γ/γ' Co-base superalloys with microstructures similar to Ni-base superalloys can be generated. This new class of high temperature materials shows promising properties but is still in its early stages of development. In this talk the positive aspects of Co as base material will be discussed and the microstructures as well as the thermo-physical, mechanical and oxidation properties of these new γ/γ' Co-base superalloys will be presented and compared with Ni-base superalloys.

MM 37.2 Wed 12:00 H26

Microstructure and mechanical properties of the ductile multicomponent Ti-based alloys — •Ilya Okulov[1,2], Simon Pauly[1], Uta Kühn[1], Tom Marr[1,2], Jens Freudenberger[1,3], Juliane Scharnweber[3], Carl-Georg Oertel[4], Werner Skrotzki[4], Ludwig Schultz[1,2], and Jürgen Eckert[1,2] — [1]IFW Dresden, 01171 Dresden, Germany — [2]TU Dresden, Institute of Material Science, 01062 Dresden, Germany — [3]TU Bergakademie Freiberg, Institute Of Materials Science, 09599 Freiberg, Germany — [4]TU Dresden, Institute of Structural Physics, 01062 Dresden, Germany

The decreasing volume fraction of intermetallic phases in nano/ultrafine-grained Ti-based alloys results in significant changes of the plasticity in tension. The Ti-based alloys were designed based on Ti66Nb13Cu8Ni6.8Al6.2 reported by Kuhn[1] and prepared by non-equilibrium processing under high cooling rates. The microstructure of these alloys consists of a dendritic bcc β-Ti solid solution and fine intermetallic phases, which precipitate in the interdendritic regions. The volume fraction of the strong but brittle intermetallic compounds significantly decreases with slight decreases in the Cu and Ni content. Consequently, the failure mechanism in tension changes from cleavage to shear fracture. The Ti71.8Nb14.1Cu4Ni3.4Al6.7 alloy demonstrates already in the as-cast state a pronounced tensile ductility of about 5.2%.

This work has been supported by the European Union and the Free State of Saxonia in the framework of ECEMP, contract no. 13853/2379.

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MM 37.3 Wed 12:15 H26

Kinetic processes in copper bi- and tricrystals — •Isabelle Binkowski[1], Jörn Leuthold[1], Matthias Wegner[1], Martin Peterlechner[1], Shashank Shekhar[2], Alex King[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]School of Materials Engineering, Purdue University, 501

Northwestern Avenue, West Lafayette, IN 47907-2044, USA

Grain boundaries (GBs) and their junctions often define properties of polycrystalline materials and have a dramatic influence on diffusion and plastic behavior. Owing to the high density of grain boundaries included in polycrystalline materials and especially nanocrystalline materials, investigation of kinetic processes in this type of defect are of fundamental interest. Heading towards nanostructured materials one has to focus also on triple junctions (TJs) since their volume fraction and thus their influence on materials' properties rise. In the present investigation, a near special $\Sigma5$:$\Sigma5$:$\Sigma25$ copper tricrystal is utilized for examining the properties of a triple junction with defined orientations of grains and defined misorientations across the grain boundaries. The mass transport properties of the tricrystal are investigated using the radiotracer method with the 110mAg isotope. The kinetics of outdiffusion from the triple junction into the neighboring grain boundaries are carefully measured by preparing proper bicrystal samples. Additionally, tensile tests including plastic deformation of several percent are performed and the digital image correlation technique is applied to measure the strain fields in the immediate vicinity of GBs and TJs.

MM 37.4 Wed 12:30 H26

Homogeneity and time dependent behavior of high pressure torsion processed copper — •Jörn Leuthold, Matthias Wegner, Sergiy Divinski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Muenster, 48149 Münster, Germany

The presence of a high defect density in the form of dislocation networks and high and low angle grain boundaries affects the plastic behavior of materials processed by severe plastic deformation . With a decrease of grain size into the sub-micrometer range, dislocation-grain boundary interactions are of increased significance for the accommodation of externally applied stresses. For this study several samples were produced by high pressure torsion, where, under a hydrostatic pressure of several GPa, large shear strains can be employed by a rotating die. Characteristic for this process is a non uniform plastic flow, since shear strain and velocity depend on the distance from the axis of rotation. As a result, an inhomogeneous microstructure is produced. After preparation, the samples were tested by nanoindentation, where, in addition to the hardness, the time dependent properties were analyzed by implementing a holding phase of 300 sec at the maximum load. Electron back-scatter diffraction was used to link the observed features of the microstructure to the results of the nanoindentation measurements.

MM 37.5 Wed 12:45 H26

Size effects of the mechanical properties of copper thin films investigated by bulge tests — •Jan Philipp Liebig, Benoit Merle, and Mathias Göken — Department of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, Germany

Plane-strain bulge testing was used to study extrinsic as well as intrinsic size effects on the mechanical behavior of thin copper films. Films of various thicknesses ranging from ˜ 100 to 1000 nm were magnetron sputter deposited on freestanding silicon nitride membranes. After heat treatment under vacuum a highly twinned microstructure is obtained. Reactive ion etching was used to remove the silicon nitride layer, in order to produce free-standing Cu-membranes. Freestanding as well as passivated Cu-films were investigated in the bulge test. From the load-deflection data, equivalent uniaxial stress-strain diagrams were calculated, allowing a reliable measurement of the yield strength and work hardening coefficients of the specimens. The relative influences of the film thickness, presence of a substrate, and microstructure as characterized by Focused Ion Beam (FIB) and Electron Backscatter Diffraction (EBSD) will be discussed in the presentation.

MM 38: Topical Session: Fundamentals of Fracture - Atomistic Modelling

Time: Wednesday 15:00–16:15 Location: H4

Topical Talk MM 38.1 Wed 15:00 H4

Modelling fracture scattering by defects in brittle crystals — •Alessandro De Vita, James Kermode, Giovanni Peralta, Marco Caccin, and Zhenwei Li — King's College London, Physics Department, Strand, London WC2R 2LS, United Kingdom

We present the results of an atomistic modelling investigation of crack-defect interaction, using the "Learn On The Fly" (LOTF) hybrid multi-scale simulation scheme [1]. The scheme is particularly well-suited to incorporate machine-learning (ML) approaches based on the predictive inference of atomic forces, and has been previously used to model both "intrinsic" crack propagation instabilities [2] and the interaction of propagating cracks with defects such as dislocations and implanted ions [3].

Here, taking as a target system B-doped ultra-pure Si samples, we provide theoretical and experimental evidence suggesting that contrary to common wisdom, propagating cracks can be deflected by hitting a single, isolated impurity atom, yielding predictable patterns of macroscopic roughness on the cleavage surface.

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MM 38.2 Wed 15:30 H4

Atomic scale modeling of damage evolution in high temperature ceramics — •Yuriy Natanzon, Denis Pilipenko, and Heike Emmerich — Lehrstuhl für Material und Prozessimulation, Universität Bayreuth, Nürnberger Straße 38, 95448 Bayreuth, Bayern

The fracture phenomenon is a major challenge for solid state physics and material science. Modelling of damage evolution is crucial for the design of advanced materials such as high temperature ceramics, which receive more attention due to increased demand for materials for extreme environments. Due to the resulting high thermal shock resistance, carbon is used in more than 40% of all fire-proof products worldwide to adjust their thermomechanical and chemical properties. For the development of "cleaner" fire-proof parts and the consequential avoidance of carbon, it is essential to understand how other materials can tailored to reach a comparable thermal shock resistance even under today's higher thermal shock stresses.

Here we present the results of atomic scale modeling of propagation of microcracks in such fire-proof ceramics by means of classical molecular dynamics with various semi-empirical interatomic potentials. The dependence of direction of crack and its speed on the various crystal orientations as well as the loading regime is calculated. and the role of charge transfer on the crack dynamics is analysed.

MM 38.3 Wed 15:45 H4

Atomistic Simulations of Cracks in α-Iron: 2D vs. 3D — •Johannes J. Möller and Erik Bitzek — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute of General Materials Properties, Martensstr. 5, 91058 Erlangen, Germany

Atomistic simulations play a crucial role in advancing our understanding of the crack tip processes taking place during fracture. As with all atomistic simulations, the results depend critically on the model of atomic interaction and on the boundary conditions. Here we present a systematic study of seven different embedded atom method (EAM) potentials applied to mode I cracks in α-iron and compare the results of straight crack fronts in quasi-two-dimensional (2D) set-ups with curved crack fronts in three-dimensional (3D) set-ups.

Infinitely long, straight crack fronts were studied in a cylindrical geometry where the atoms are displaced according to the anisotropic linear-elastic solution and periodic boundary conditions are applied along the crack front direction. Comparison of the fracture behavior and critical stress intensity factors to experimental data allows us to rank the potentials according to their capability to realistically model fracture in α-iron. The results of these quasi-2D simulations are compared to large-scale 3D molecular statics and -dynamics simulations of penny shaped cracks. The plastic deformation mechanisms and changes in crack morphology are analyzed in detail and related to the curvature of the crack front and the 3D simulation set-up. The results highlight the importance of 3D models to study microstructurally short cracks.

MM 38.4 Wed 16:00 H4

Studying Short Cracks with a 3D Multiscale Model — •Steffen Brinckmann — Max Planck Institut für Eisenforschung

Grooves and notches act as initiation sites for short cracks, which grow into size and lead to a failure of the structure. To understand the fundamentals of short cracks, a multiscale model is warranted, which accounts for fracture on the atomistic level, while covering plasticity on a micrometer length scale.

Multiple multiscale models exist, which cover these intrinsic length scales: atomistic separation by Molecular Dynamics and micrometer plasticity by Dislocation Dynamics. In the past, these models were restricted to two dimensional configurations, which limited their applicability and altered the fundamental deformation behavior of the metal.

In this contribution a three-dimensional, concurrent multiscale model of Molecular and Dislocation Dynamics is introduced and applied to microscale plasticity around a short penny-shaped notches, which is located at the free surface. Since this contribution is the first-time presentation of the three-dimensional model AtoDis, a full description of the mechanical model, especially at the interface is given.

The talk will close with remaining challenges in the current model and a general discussion about model verification, which is applicable to multiple of the currently developed multiscale models.

MM 39: Computational Materials Modelling - Transport, Excitations, Time Dependence I

Time: Wednesday 15:00–16:15 Location: H24

MM 39.1 Wed 15:00 H24

Thermal conductivity of graphene from first principles — •Andrea Cepellotti[1], Nicola Bonini[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The thermal conductivity of graphene is computed from the Boltzmann equation for phonon transport, where phonons are treated semiclassically and vibrational properties and anharmonic scattering rates are obtained from density-functional perturbation theory. We show that the commonly used single-mode relaxation time approximation (SMRTA) is not accurate, even at high temperatures, due to the unusually large number of normal scattering processes compared to umklapp ones. By relaxing the SMRTA and solving the Boltzmann equation self-consistently [1] we are able to recover excellent agreement with experimental data [2]. We also rationalize the variations in experimental measurements as an effect of sample finite dimensions, due to the large contributions coming from long wavelength phonons. As pointed out in previous simulations [3], we underline the critical role of strain in the renormalization of the out-of-plane acoustic modes and quantify its effects. Finally, we show how strain and sample size can be used to tune thermal conductivity in graphene over a large range of values.

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MM 39.2 Wed 15:15 H24

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, techniques that rely on the harmonic approximation are no longer valid, while standard non-equilibrium molecular dynamics methods require huge temperature gradients that lead to deviations from Fourier's law. The Green-Kubo method [1], which does not suffer from these shortcomings, involves the assessment of the thermal conductivity from the auto-correlation of the heat flux in equilibrium. In classical MD, the heat flux is computed from the energetic contributions of the individual atoms; we show that the Green-Kubo approach can be reformulated in terms of the energy and stress densities [2], which are directly accessible in DFT calculations. This approach leads to a unique definition of the heat flux that does not rely on any partitioning scheme for the total energy. We critically discuss the computational cost, the accuracy, and the applicability of this approach by investigating the thermal conductivity for oxides and semiconductors with low thermal conductivities.

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MM 39.3 Wed 15:30 H24

Ab-initio study of q-dependent screening parameters and effective plasma frequencies in simple metals — •Steffen Kaltenborn and Hans Christian Schneider — University of Kaiserslautern, 67653 Kaiserslautern, Germany

We present results of an ab-initio study of the dielectric function $\varepsilon(\mathbf{q},\omega)$ in the RPA approximation together with energies and wave functions from density functional theory [1,2]. We have implemented the linear tetrahedron method for the computation of the dielectric function and therefore do not need to use a phenomenological broadening of the energy conserving delta function. From the dielectric function we determine the effective plasma frequency Ω and the static screening wave number κ for the simple metals aluminum, silver and copper. In all metals, we find a pronounced deviation from the parabolic dispersion $\Omega \propto q^2$ of the plasma frequency that is often assumed [3]. In particular, for aluminum the effective plasma frequency decreases with finite $\mathbf{q}$-vectors until it reaches the electron-pair continuum. We also discuss the influence of the spin mixing on plasma frequency and screening wave number. Last, we compare our results with measurements [4] and with computed results using a finite broadening in the RPA dielectric function, as implemented in current DFT codes [1,2].

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MM 39.4 Wed 15:45 H24

Spectral density and metal-insulator phase transition in Mott insulators within RDMFT — •Sangeeta Sharma, John Kay Dewhurst, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We present a method for calculating the spectrum of periodic solids within reduced density matrix functional theory. This method is validated by a detailed comparison of the angular momentum projected spectral density with that of well established many-body techniques, in all cases finding an excellent agreement. The physics behind the pressure induced insulator-metal phase transition in MnO is investigated. The driving mechanism of this transition is identified as increased crystal field splitting with pressure, resulting in a charge redistribution between the Mn eg and t2g symmetry projected states.

MM 39.5 Wed 16:00 H24

Embedded impurity method applied to positron annihilation lifetime simulations — •Martin Offenberger[1], John Banhart[2], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz-Zentrum Berlin für Materialien und Energie

Within the Korringa-Kohn-Rostoker (KKR) framework of solid state simulations, the embedded impurity method is an efficient alternative to the supercell ansatz to describe impurity systems like substituted atoms or vacancies. This approach allows to study electronic properties and interactions between different alloying elements and vacancies on an atomic level.

As positrons are strongly attracted to vacancies and to a lesser degree to certain types of impurities, this method is of great advantage for positron annihilation studies.

We demonstrate the implementation of structural relaxation around impurities into the Munich SPRKKR band structure program package. Corresponding results for positron annihilation lifetimes of impurity-vacancy cluster systems embedded into Aluminium will be presented.

In addition the potential models (ASA or full potential) used within KKR calculations and their influence on electron and positron calculations for embedded impurity systems will be discussed.

MM 40: Topical Session: TEM-Symposium - In-Situ I

Time: Wednesday 15:00–16:15 Location: H25

Topical Talk MM 40.1 Wed 15:00 H25

The kinetics of nanowire growth as seen by ultra-high vacuum transmission electron microscopy — •Frances M. Ross — IBM T. J. Watson Research Center, Yorktown Heights, NY, USA

Nanowires formed from semiconducting materials have exciting applications in electronics and optoelectronics, solid state lighting, sensing, and energy storage and conversion. These applications arise from the ability to control crystal structure and composition with great precision, for example to form abrupt heterointerfaces or specific polytypes. Here we show how direct, in situ observations using ultra-high vacuum transmission electron microscopy can help us understand the mechanisms of nanowire growth. Nanowires are formed by flowing precursor gases onto a heated sample containing catalytic particles. For Si and Ge nanowires, this allows us to visualise the ledge-flow growth mechanism directly and explore the relationship between catalyst phase and interface formation. Here, we focus on III-V nanowires, specifically GaP, where in situ measurements show unexpected changes in growth rate from one atomic layer to the next that depend on local defects. We can understand the differences in kinetics by considering the pathways and chemical potentials of the species involved. In situ microscopy therefore provides a unique view into growth and structural control in these complex and versatile nanomaterials.

MM 40.2 Wed 15:30 H25

Birth, motion, interaction, and annihilation of dislocations in graphene at the atomic scale — •Ossi Lehtinen[1,2], Simon Kurasch[1], Arkady V. Krasheninnikov[2,3], and Ute Kaiser[1] — [1]Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm — [2]Department of Physics, University of Helsinki, Finland — [3]Department of Applied Physics, Aalto University

Dislocations, one of the key concepts in materials science, govern the mechanical properties of any material. Thus, understanding their life cycle, from creation to annihilation via motion and interaction with other dislocations, point defects, and surfaces is of fundamental importance. Unfortunately, atomic scale investigations of dislocation evolution in a bulk object are well beyond the spatial and temporal resolution limits of current characterization techniques, and therefore such studies have long been reserved for computer simulations and analytical theory. Here, we overcome the experimental limits by investigating a two-dimensional material, graphene, in an aberration-corrected transmission electron microscope, exploiting the impinging energetic electrons both to image and stimulate atomic scale morphological changes in the material. The resulting transformations are followed *in-situ*, showing the full life cycle of a dislocation from birth to annihilation. Our experiment, combined with atomistic simulations, reveals the underlying mechanism of interaction to be out-of-plane buckling, which leads to markedly long-range interactions of the defects.

MM 40.3 Wed 15:45 H25

Superdislocation characterization by means of large angle convergent beam electron diffraction (LACBED) — •Julian Müller and Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg

Superdislocations (SD) play an important role for the mechanical properties of ordered intermetallic compounds. For instance, in Ni base superalloys the formation of SDs and their glide/climb across the ordered γ' phase are key elementary processes in high-temperature creep. A key step of the microscopic characterization of dislocations in the transmission electron microscope is the determination of the Burgers vector (BV) which is typically performed by identifying two-beam conditions for which the dislocation is invisible. However, in the case of SDs difficulties in the conventional BV analysis often arise due to pronounced residual contrast. In this work we demonstrate that LACBED is well suited for reliable BV analysis of SDs even in cases where the conventional analysis fails. We confirm that SDs with BVs of type a<110> and a<100> coexist in high temperature crept Ni-base superalloys, which means that the SDs are composed of partials with identical or different BVs of type a/2<110>, respectively. We use weak-beam dark field imaging and STEM tomography to reveal the corresponding splitting of the SDs into partials.

The authors gratefully acknowledge the DFG RTG 1229 and SFB/TRR 103 for financial support and L. Agudo and G. Eggeler from Ruhr University Bochum for providing the samples.

MM 40.4 Wed 16:00 H25

Real-time observation of grain boundary migration in graphene with atomic resolution — •Carl Krill[1], Simon Kurasch[2], Dana Zöllner[3], Ossi Lehtinen[4], Jani Kotakoski[4], Arkady Krasheninnikov[4,5], and Ute Kaiser[2] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Group of Electron Microscopy of Materials Science, Ulm University, Germany — [3]Institute of Experimental Physics, University of Magdeburg, Germany — [4]Department of Physics, University of Helsinki, Finland — [5]Department of Applied Physics, Aalto University, Finland

Grain growth in polycrystalline solids is a materials science manifestation of survival of the fittest, with individual grains seizing every opportunity to steal atoms away from their neighbors. What fate befalls an atom caught in this bitter struggle, subject to the nefarious desires of two or even three neighboring grains? Until now, it has been impossible to answer this question definitively, as experimental techniques lack the spatial and temporal resolution needed to capture atomic-level dynamics during grain growth. By irradiating polycrystalline graphene with electrons in an aberration-corrected TEM, however, we show that grain growth can be studied for the first time experimentally on an atom-by-atom basis. We can watch configurational fluctuations in the boundary core region average out over time, resulting in mesoscopic translation in the direction of local curvature. The extreme case of a small graphene grain completely embedded within a larger one represents an ideal model system for testing the validity of atomic-scale computational models for grain growth.

MM 41: Mechanical Properties II

Time: Wednesday 15:00–16:15 Location: H26

MM 41.1 Wed 15:00 H26

Investigation of residual stress in straightened steel pipes with diffraction methods — •Sascha Raatz[1], Heike Oppermann[1], Peter Staron[2], Michael Hofmann[3], Michael Kaack[4], and Katharina Theis-Bröhl[1] — [1]University of Applied Sciences Bremerhaven, 27568 Bremerhaven — [2]Helmholtz-Zentrum Geesthacht (HZG), 21502 Geesthacht — [3]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) , 85747 Garching — [4]Salzgitter Mannesmann Forschung GmbH (SZMF) , 47259 Duisburg

In our study we compare several non-destructive evaluation methods to determine the residual stress in steel components due to a demand from the industry for reliable on-site testing. The chosen samples are low-alloy steel pipes with different levels of a straightening process which leaves a visible helix on the surface. We used synchrotron diffraction at the HEMS beamline at DESY and neutron diffraction at STRESS-SPEC at the FRM II to get absolute values for the residual stress in the bulk of our samples. The samples have a wall-thickness of 4 mm and the measurements show the highest residual stresses approximately 1 mm under the surface. The residual stresses correlate with the levels of straightening and change their values up to 400 MPa through the wall-thickness.

We acknowledge funding by BMBF, DESY, FRM II and cooperation with HZG. The samples were provided by our industrial partner SZMF.

MM 41.2 Wed 15:15 H26

Influence of hydrogen on the defect structure in metals subjected to plastic deformation — •Martin Deutges[1], Inga Knorr[1], Hans Peter Barth[1], Yuzeng Chen[2], Christine Borchers[1], Cynthia Volkert[1], and Reiner Kirchheim[1,3] — [1]Institut für Materialphysik, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]State Key Lab of Solidification Processing, Northwestern Polytechinical Univeristy, Xi'an, China — [3]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

The interaction between dissolved atoms and crystal defects can be studied on specific model systems.

Hydrogen enhances the formation and the mobility of dislocations. This can be demonstrated by palladium which is cold rolled with and without hydrogen content. The presence of hydrogen markedly increases the dislocation density. TEM investigations show that the arrangement of dislocations changes with hydrogen concentration.

Another experiment is the deformation of vanadium micropillars. At low hydrogen concentrations, the pillars deform on a few discrete slip planes generating serrations, and at higher concentrations the pillars deform to a barrel-like shape.

These experiments can be analyzed using the defactants concept. The basis of the defactants concept is the assumption that a decrease of the overall free energy by the segregation of solute atoms to a defect can be ascribed to a decrease in the defect formation energy.

MM 41.3 Wed 15:30 H26

Structure and thermal stability of severe plastically deformed Cu84Al16 — •Nazar Ibrahim, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, Muenster, Germany

Severe plastic deformation (SPD) is an effective tool for production ultrafine grained materials with extraordinary mechanical properties. High strength and relatively good ductility are attributed to their fine microstructure. In this work, structure modification by high pressure torsion (HPT) and the thermal stability of the resulting microstructure are investigated for the Cu*16 at.% Al alloy . For this alloy, a propensity for the formation of five-fold twinning has recently been reported [X.H. An, et al., Scripta Materialia 64 (2011) 249]. Disks of thickness of 0.8 mm and diameter of 10 mm were processed via HPT for 2,5,10 and 20 revolutions at room temperature using an imposed pressure of 6.0 GPa and rotational speed of 1 rpm. Structural and thermal analyses were carried out using X-ray diffraction, transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). The DSC experiments using constant heating rates showed two exothermic peaks in the temperature range from 30°C to 450°C. After HPT a highly distorted structure was observed, including dislocations, fragmented grains and twins. The twin thickness in Cu84Al16 has been determined from TEM observation to be in the range of 2 to 6 nm. These small thicknesses are in agreement with the low stacking fault energy of the alloy. The results are discussed with respect of the reported five-fold twinning in this alloy.

MM 41.4 Wed 15:45 H26

Mechanical Spectroscopy on deformed Al-Mg-Si (AA6061) alloy: Characterization of interactions between solute atoms, precipitates and dislocations — •Jens Bernhardt and Hans-Rainer Sinning — Institut für Werkstoffe, Technische Universität Braunschweig, Germany

Industrially used alloy AA 6061 shows a great variety of microstructural effects. In homogenized samples formation of solute clusters starts during storing at room temperature (RT). At higher temperatures a complex precipitation sequence takes place changing microstructural state and therefore mechanical properties of the alloy. In addition mobility of solute atoms is increasing with increasing temperature. Since dynamics of dislocations are governed by microstructural material state and by interaction with solute atoms, characteristics of dislocation dynamics are changing with temperature. In order to investigate the interaction of dislocations with precipitates and solute atoms, temperature dependent internal friction (TDIF) between 80 and 292 K was measured, after different thermal treatments and plastic deformation at 80 K and 292 K respectively, using the vibrating-reed technique with small strain amplitudes between about 10^{-6} and 10^{-5}. Interaction between solute atoms and dislocations can also be affected by these small strains, hence TDIF was measured at both high (10^{-5}) and low (10^{-6}) strain amplitude. The results are discussed regarding applied deformation, strain amplitude and thermal treatment in order to characterize the dynamics of dislocations in AA 6061 and related aspects of the Portevin-Le Chatelier effect.

MM 41.5 Wed 16:00 H26

The influence of different Equations of State on the calculation of elastic properties — •Claudia Loose and Jens Kortus — TU Bergakademie Freiberg, Fakultät für Chemie und Physik, Leipziger Str. 23, 09599 Freiberg

Equations of state (EOS) describe the behavior of solids under compression and are widely used in geophysics and high-pressure research. However there is no general thermodynamic basis for the correct form of a solid state EOS, hence there are many different EOS in use. Here we present density functional calculations of different AlN and SiO_2 phases up to very high compressions V/V_0=0.58. We use seven different EOS to fit the equilibrium volume V_0, the bulkmodulus B and pressure derivative of the bulkmodulus B' using the obtained energy-volume data. A comparison of the elastic properties obtained from these fits revealed significant dependence on the regarded EOS.

MM 42: Topical Session: Fundamentals of Fracture - Continuous Models

Time: Wednesday 16:30–17:45 Location: H4

Topical Talk MM 42.1 Wed 16:30 H4

Configurational Mechanics: A Continuum Approach to Model Fracture and Defects — •Paul Steinmann — Chair of Applied Mechanics, University Erlangen-Nuremberg, Germany

Configurational mechanics is a branch of continuum modelling that allows to model fracture and defects (such as single and distributed dislocations, interfaces, vacancies, etc) based on concepts from continuum field theories. The key notion is hereby the configurational force that is dual (in terms of the dissipation power) to the motion of these kind of defects relative to the ambient material. This is clearly opposite to the common notion of forces that may be considered as being energetically dual to the motion of material relative to the ambient space. The talk will highlight especially the roots of concepts from fracture mechanics in continuum modelling. Configurational mechanics then allows to include straightforwardly various modelling options such as coupled problems or lenght scale dependent models. Especially at the micro and nano scale the material response in general and the fracture behavior in particular become decisively dependent on the ratio of lengths characterizing the dimension of a specimen and the dimension of the materials micro structure. These effects may be captured by gradient and/or surface enhanced continuum models, both having direct consequences within configurational mechanics.

MM 42.2 Wed 17:00 H4

Modeling of planar cracks in 3D elastic media considering the effects of surface elasticity by using FEM - SGBEM coupling — •Binh Thai Nguyen[1], Jaroon Rungamornrat[1], Teerapong Senjuntichai[1], and Anil C. Wijeyewickrema[2] — [1]Department of Civil Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok 10330, Thailand — [2]Department of Civil and Environmental Engineering, Tokyo Institute of Technology, Tokyo 152-8552, Japan

A computationally efficient and accurate numerical technique having the ability to model isolated planar cracks in three-dimensional linear elastic media considering the effects of surface elasticity is presented. The governing equations are formulated based on the classical theory of linear elasticity for the bulk and Gurtin-Murdoch surface elasticity model for the crack surfaces. The resulting system of equations is then solved numerically by using the FEM-SGBEM coupling procedure. Application of the technique to the stress analysis of nano-crack problems are also presented for some selected cases to study the nano-scale influence and size-dependency behavior.

MM 42.3 Wed 17:15 H4

On the Propagation of two en passent cracks upon mutual interaction: A phase field study — •Martin Lautenschläger,

Michael Fleck, Denis Pilipenko, and Heike Emmerich — Materials and Process Simulation, University of Bayreuth, Germany

A phase field model for the simulation of crack propagation in brittle materials is applied to the problem of two mutually interacting "en passent" cracks. Thereby, crack growth is described as a first order phase transformation process, where the solid parent phase transforms into an infinitely weak "broken" phase, driven by elastic energy dissipation. We discuss the problem of "en passent" cracks in a two dimensional plain strain geometry, subjected to a constant uniaxial pulling velocity of mode I type. Our model reproduces a number of basic features that are also observed in corresponding experimental setups: Initially, when the two cracks propagate independently, they approach each other along straight paths. Then, during the early stage of the mutual interaction and for certain geometrical circumstances the principle of local symmetry may even force the cracks to turn slightly away from each other. When the line connecting the two crack tips alines with the pulling direction, the two cracks curve towards each other upon mutual tip-tip interaction until each crack tip reaches the other's crack tail, finally releasing a lenticular fragment. Here, we investigate the crack propagation dynamics as well as the chosen crack paths as a function of all relevant physical dependences, such as the pulling velocity, the materials Poisson ratio and so forth.

MM 42.4 Wed 17:30 H4

Simulation of damage accumulation in slip bands and their influence on the resonant behavior in the very high cycle fatigue (VHCF) regime — •Philipp-Malte Hilgendorff[1], Andrei Grigorescu[2], Martina Zimmermann[3], Claus-Peter Fritzen[1], and Hans-Jürgen Christ[2] — [1]Institut für Mechanik und Regelungstechnik - Mechatronik, Universität Siegen, Germany — [2]Institut für Werkstofftechnik, Universität Siegen, Germany — [3]Institut für Werkstoffwissenschaft, Technische Universität Dresden, Germany

The service life of structural components under very high cycle fatigue loading is mainly determined by the period of fatigue crack initiation and thus the localization of plastic deformation. By means of a new approach the characterization of the damage accumulation in the VHCF regime is based on the resonant behavior of the specimen. The resonant behavior of a metastable austenitic stainless steel (AISI304) is studied experimentally in the VHCF regime and shows a distinct transient characteristic. To obtain a physically-based understanding of this characteristic, a microstructural simulation model is proposed which accounts for the damage mechanisms of slip bands. The implementation of the simulation model into a numerical method allows the investigation of the damage accumulation in a simulated microstructure. The numerical method used in this study is the two-dimensional (2-D) boundary element method which is based on two integral equations. Results show that simulation of slip bands is in good agreement to microscopic observations and that plastic deformation in slip bands influences the transient characteristic of the resonant behavior.

MM 43: Computational Materials Modelling - Transport, Excitations, Time Dependence II

Time: Wednesday 16:30–17:45 Location: H24

MM 43.1 Wed 16:30 H24

On low-energy electronic excitations in the $Ti_{1-x}Al_xN$-system — •Simon Lamowski, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany

Layered structures of $Ti_{1-x}Al_xN$ were characterized by electron energy-loss spectroscopy scanned along a direction perpendicular to the interface. By means of ab initio Density Functional Theory (DFT) calculations using the full potential linearised augmented plane wave (FP-LAPW) method as implemented in the Elk code [1] we investigate structural and electronic factors which influence the EELS up to an energy-loss of 60 eV.

Further, we go beyond standard DFT by solving the Bethe-Salpeter-Equation [2] to obtain the free parameters for the long range contribution exchange - correlation kernel [3] for time dependent DFT (TDDFT). This allows to use the TDDFT with lower computational cost to calculate EELS for supercells with defects and layers.

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[3] Botti S, et al. Physical Review B; 2005;72(12):125203.

MM 43.2 Wed 16:45 H24

Real-time evolution in solids on the attosecond time scale — Kevin Krieger, •John Kay Dewhurst, Sangeeta Sharma, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We report on the first implementation of real-time evolution in solids in an all-electron code. Starting from the Kohn-Sham ground-state, a short laser pulse is applied to the crystal in the form of a time-dependent vector potential. The subsequent time-evolution is performed by an efficient and strictly unitary algorithm using an instantaneous LDA or GGA as the TDDFT functional. This allows the investigation of time-evolution well beyond the linear-response regime. The method is then applied to several materials in order to understand phenomena such as the spin-dynamics processes in magnetic metals. We further discuss how the time-dependent Kohn-Sham equations can be coupled to Maxwell's equations and discuss strategies for developing associated functionals.

MM 43.3 Wed 17:00 H24

Robust dynamical decoupling with concatenated continuous driving — •Kay Jahnke[1], Jian-Ming Cai[2], Boris Naydenov[1], Rainer Pfeiffer[1], Liam McGuinness[1], Fedor Jelezko[1], Martin Plenio[2], and Alex Retzker[3] — [1]Institut für Quantenoptik, Uni Ulm — [2]Institut für Theoretische Physik, Uni Ulm — [3]Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

The loss of coherence is one of the main obstacles for the implementation of quantum information processing. The efficiency of dynamical decoupling schemes, which have been introduced to address this problem, is limited itself by the fluctuations in the driving fields which will themselves introduce noise. We address this challenge by introducing the concept of concatenated continuous dynamical decoupling, which can overcome not only external magnetic noise but also noise due to fluctuations in driving fields. We show theoretically that this approach can achieve relaxation limited coherence times, and demonstrate experimentally that already the most basic implementation of this concept yields an order of magnitude improvement to the decoherence time for the electron spin of nitrogen vacancy centers in diamond. The proposed scheme can be applied to a wide variety of other physical systems, including trapped atoms and ions and quantum dots, and may be combined with other quantum technologies challenges such as quantum sensing and quantum information processing.

MM 43.4 Wed 17:15 H24

photo-emission spectroscopy study for the tautomeric populations of DNA and RNA nucleobases: an application of koopmans' compliant functionals. — •ngoc linh nguyen[1], giovanni borghi[1], Nicola Marzari[1], Andrea Ferretti[2], and Ismaila Dabo[3] — [1]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne — [2]CNRNANO, Universie di Modena e Reggio Emilia — [3]CERMICS, Universite Paris-Est

We study the structural and photo-electron properties of five DNA and RNA nucleobases - guanine (G),adenine (A), cytosine (C), thymine (T), and uracil (U), using either Perdew-Zunger self-interaction corrections [1] to density-functional theory, or Koopmans' compliant functionals [2]. A simple method for simulating photoemission spectra of molecules is also implemented, based on a plane-wave approximation for the final states to account for the transmission matrix. Finally, the experimental photoemission spectra are modelled by summing the individual spectra of each tautomer, weighed by the Boltzmann population ratios for the tautomers. Our calculations show that Koopmans' compliant functionals provide vertical ionization energies compatible with the values computed by high-accuracy quantum chemistry methods, and spectra that are in remarkable agreement with experimental results.

[1] J. P. Perdew and Alex Zunger, Phys. Rev. B 23, 5048 (1981).
[2] I. Dabo1, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M.

Cococcioni, Phys. Rev. B 82, 115121 (2010).

MM 43.5 Wed 17:30 H24

Nuclear quantum effects in *ab initio* IR spectra of water clusters and peptides — •Mariana Rossi[1], Volker Blum[1], Carsten Baldauf[1], Michele Ceriotti[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Oxford, UK

Nuclear quantum effects (NQE) are important in biochemical-related processes (e.g., Ref. [1]), but still present a challenge for *ab initio* (AI) treatments, especially regarding dynamical quantities. We have recently implemented two features in the all-electron code FHI-aims [2], that allow for an efficient and accurate estimation of NQE from an AI perspective: (i) Generalized Langevin Equation based thermostats (GLE) [3] that can approximate NQE, and (ii) an interface to a wrapper code [4] that performs path integral (PI) ring-polymer molecular dynamics (RPMD) and centroid molecular dynamics (CMD). With these methodologies, we quantify NQE effects in IR spectra of protonated water clusters and protonated peptides. IR spectra obtained from classical AI microcanical simulations started from GLE-thermostated runs successfully approximate NQE for small protonated water clusters. However, we provide a simple physical reason why for large and floppy peptides this approximation can fail even qualitatively, making necessary the explicit inclusion of NQE. Using AI PI based methods we can also reproduce key features of the IR spectra of Zundel-like cations observed experimentally. [1] Masgrau *et al.*, Science 312, 237 (2006) [2] Blum *et al.*, CPC 180, 2175 (2009); [3] Ceriotti, Bussi, Parrinello, JCTC 6, 1170 (2010); [4] Ceriotti, More, Manolopoulos, private communication.

MM 44: Topical Session: TEM-Symposium - In-Situ II

Time: Wednesday 16:30–17:45 Location: H25

MM 44.1 Wed 16:30 H25

Nanoscale investigation of metal-induced crystallization (MIC) and related mass transport by in-situ TEM/STEM — Balaji Birajdar[1], Simon Kraschawski[1], Benjamin Butz[1], Tobias Antesberger[2], Martin Stutzmann[2], and •Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaft, Universität Erlangen-Nürnberg — [2]Walter Schottky Institut and Physics Department, Technische Universität München

The MIC process enables fabrication of thin polycrystalline Si films at relatively low temperature ($< 450°C$) making it highly promising for thin film photovoltaics. The microscopic mechanism of materials transport during the layer exchange is still largely unknown. Here the microstructure of a-Si/metal/Quartz stacks, in-situ annealed at 450-530 °C, have been investigated at different length scales by combining optical microscopy and analytical TEM/STEM [1]. In particular Ag metal layer was used to directly visualize the material transport by Z-contrast imaging in STEM due to the large difference in atomic numbers of Ag and Si. Like in Al induced crystallization, Si grains are nucleated in the original Ag layer and grow dendritically as the smaller Ag grains were preferentially replaced by Si. The replaced Ag was observed to concentrate over the larger Ag grains replacing the a-Si which appears to diffuse out. Thus in contrast to Al induced crystallization a continuous Si film could not be formed, indicating the importance of Ag grain size distribution. [1] B. Birajdar, T. Antesberger, M. Stutzmann, E. Spiecker, Scripta Mater. 66, 550 (2012).

Topical Talk MM 44.2 Wed 16:45 H25

In-situ environmental TEM studies of oxide electro-catalysts — •Christian Jooss[1], Stephanie Raabe[1], Daniel Mierwaldt[1], Jim Ciston[2], Matthé Uijttewaal[3], Jörg Hoffmann[1], Peter Blöchl[3], and Yimei Zhu[4] — [1]Inst. of Materials Physics, University of Goettingen, Germany — [2]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, USA — [3]Inst. of Theoretical Physics, Technical University of Clausthal, Germany — [4]Dep. of Cond. Mat. Phys., Brookhaven National Laboratory, USA

In-situ studies of catalysts under operation conditions are of high scientific interest since their atomic and electronic structure in their active state may fundamentally differ from that in equilibrium. In addition, reactions in the vapor phase can hardly be observed. We present an in-situ ETEM study of electro-catalytic O_2 evolution during H_2O splitting based on Pr-doped $CaMnO_3$ perovskite catalysts. This materials system offer the opportunity for studies of the role of correlation effects and mixed valence physics in multi-charge transfer catalysis. We observe changes in surface and subsurface structure as well as in Mn valence in the active state during O_2 evolution. The electro-chemical processes can be controlled by application of a bias. For validation of the obtained results, the ETEM studies are complemented by in-situ X-ray absorption spectroscopy (XANES) and ex-situ cyclic voltammetry studies. This allows for deriving conclusions about the opportunities and challenges for controlled electro-chemical experiments in the ETEM. S. Raabe et al. Adv. Funct. Mater. 2012, DOI: 10.1002/adfm.201103173

MM 44.3 Wed 17:15 H25

Dynamic atomic-scale observation of catalysts in their functional state by aberration-corrected environmental transmission electron microscopy (ETEM) — •Joerg Jinschek — FEI Company, Eindhoven, The Netherlands

Currently the strong focus on energy producing and environmental protecting technologies relies on the advancement of new functional catalysts. Characterization of the state and properties as well as catalyst*s performance demands detailed dynamic atomic-scale insights while in operation conditions [1]. The implementation of differential pumping apertures in an aberration corrected TEM (FEI Titan ETEM) enables to maintain high-resolution imaging and analytical capabilities, while confining a gas environment in the close vicinity of the catalyst specimen. Atomic-scale imaging in ETEM has opened up a unique possibility to monitor heterogeneous catalysts during exposure to reactive gas environments and temperatures [2]. As an example, a catalyst composed of Au nanoparticles supported on CeO2 , active for the oxidation of carbon monoxide (CO) even below room temperature, has been examined utilizing Titan ETEM [3]. The results of in situ HRTEM experiments depict that adsorbed CO molecules cause the Au{100} facets of a gold nanoparticle to reconstruct to Au{100}-hex. The energetic favorability of this reconstructed structure has been confirmed by ab initio calculations [3]. [1] P. L. Hansen et al. Science 295, 2053 (2002); [2] J.R. Jinschek, S Helveg. Micron 43, 1156 (2012); [3] H. Yoshida, et al. Science 335, 317 (2012)

MM 44.4 Wed 17:30 H25

Electron-beam-stimulated mechanical engineering of nanoscaled amorphous silica — •Mirza Mackovic and Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy, Cauerstr. 6, 91058 Erlangen, Germany

Oxide glasses are widely used as structural and functional materials in electronic, optical, and nanoelectromechanical devices. Since amorphous silica does not show ductility at room temperature, complications arise if one considers its application in functional devices, because no shaping or re-shaping is possible without significantly rising the temperature. However, using electron-beam-assisted deformation just recently it has been demonstrated that enormous ductility and superplasticity can be achieved for nanoscaled amorphous silica, at or near room temperature [1]. This material behavior is related to the electron-beam-induced generation of structural and bonding defects, facilitating bond-switching events in the silica network and accommodating viscous flow. Using in-situ nanomechanical testing in a transmission electron microscope, we show that this electron-beam-stimulated viscous flow and shape change of nanoscaled silica is even reversible and can thus be considered for re-shaping not only once, but multiple times. Furthermore, we demonstrate that this phenomenological reversibility can be exploited for generating anisotropic glass topology by specific electron-beam-stimulated quenching under mechanical load. This offers new opportunities for fundamental studies on structure-property relations of nanoscaled glass, which have remained unexplored till now. [1] K. Zheng et al., Nature Comm. 1:24, DOI: 10.1038/ncomms1021.

MM 45: Nanomaterials - Nanospheres & Fibres

Time: Wednesday 16:30–17:45 Location: H26

MM 45.1 Wed 16:30 H26

Fabrication of transparent metal electrodes by nanosphere lithography — •Eser Metin Akinoglu, Anthony Morfa, and Michael Giersig — Freie Universität Berlin, Department of Physics, Berlin, Germany

Electrodes providing sufficient transparency and conductivity are important for high performance optoelectronic applications such as thin-film solar cells and light emitting diodes. Periodically perforated metal films provide a tunable basis to achieve high transparency while maintaining a low sheet resistance by simply changing the geometrical dimensions of the metal grid.

Nanosphere lithography is an inexpensive method to fabricate tunable transparent metal electrodes. This technique utilizes a self assembled and hexagonally close packed monolayer of colloidal polystyrene submicron particles as a lithography mask. Annealing and reactive ion etching in an oxygen plasma is used to modify the mask. Metal is then deposited and the resultant metal nanostructure shapes and dimensions are determined by the mask's negative image.

In this presentation we discuss results from transparent silver electrodes produced in this way. We demonstrate structural, electronic and optical properties of our gratings with SEM, AFM, four-point probe and optical measurements. Sheet resistances as low as 3 Ohm/Sq and an average transmissivity of 70% was achieved. Percent transmission values up to 82% are predicted by a simple geometric model promising competitiveness with transparent conductive oxides. Finally, these silver electrodes were incorporated into organic photovoltaic devices.

MM 45.2 Wed 16:45 H26

C_{58} solid materials: mechanical properties vs thermal stability — Seyithan Ulas[1], Sven Bundschuh[2], Chris Eberl[2], Henrik Hölscher[3], •Artur Böttcher[1], and Manfred Kappes[1] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Advanced Materials and Material- and Biomechanics (IAM-WBM), KIT, Germany — [3]Institute of Microstructuring Techniques, KIT, Germany

Non-IPR C_{58} cages as created by electron-impact induced fragmentation of IPR-C_{60} fullerenes have been exploited as building blocks of new materials grown by applying low energy cluster beam deposition. The material fabricated at room temperature appears to be an amorphous wide-band semiconductor, RT-C_{58}. Nanoindentation as applied to measure elastic modulus E and hardness H reveals values higher than those found for IPR-C_{60} solids: E(RT)=14.1 GPa and H(RT)=1.23 GPa. This observation is rationalized in terms of the unique functionalization of C_{58} cages by non-IPR sites which are responsible for the formation of covalently stabilized C_{58} oligomers. Annealing the RT-C_{58} films up to 1100 K results in a new material, HT-C_{58}, which exhibits considerably modified electronic and vibrational properties. Such annealing activates the mobility of the initially vdWaals-stabilized cages and consequently maximizes their coordination degree (densification and strengthening by covalent interlinking). The related molecular transformations raise the overall mechanical hardness of the material: H(HT)= 3.9 GPa, i.e. H(HT)=3 H(RT).

MM 45.3 Wed 17:00 H26

Electrical properties of different kinds of multi-walled carbon nanotubes powders — •Abdelwahab Hassan[1], Silke Hampel[1], Christian Hess[1], Anatoly Romanenko[2], Manfred Ritschel[1], Albrecht Leonhardt[1], and Bernd Buechner[1] — [1]IFW-Dresden, D-01171 Dresden, Germany — [2]Institute of Inorganic Chemistry, Novosibirsk 630090, Russia

Carbon nanotubes have attracted great interest due to their remarkable structure, electrical and mechanical properties. Among various other properties of CNTs studied so far, the electrical transport properties are still unclear and needs a lot of attention. The electrical properties are strongly dependent on the structure of the nanotubes which varied with the quality of the CNTs. Different kinds of multi-walled carbon nanotubes MWCNT were synthesised by two CVD techniques (aerosol and fixed-bed CVD).The aim of this work is to study and compare the electrical properties as a function of synthesis condition and treatments of MWCNT powders. Morphologies of these MWCNTs are studied using Scanning Electron Microscopy and Transmission Electron Microscopy. The electrical measurements were separately carried out in two temperature ranges (4-294 K and 300-570 K) by four point technique. In the high temperature range 300-570 K, the conduction was found to be thermally activated and well described by Arrhenius type behaviour. However, in the low temperature range (4-294 K),the measured data gives a good fit to variable-range hopping (VRH) and the results are interpreted using Motts (VRH) model. By using these models, various interesting electrical parameters have been calculated.

MM 45.4 Wed 17:15 H26

Quantification of curvature effects in boron and carbon nanotubes: large errors in the zone-folding method — •Hagen Eckert[1], Viktor Bezugly[1,2], Jens Kunstmann[1,3], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Division of IT Convergence Engineering, POSTECH, Pohang 790-784, Republic of Korea — [3]Department of Chemistry, Columbia University, New York NY 10027, USA

The zone-folding method is a widely used technique for computing the electronic structure of carbon nanotubes as well as of other type nanotubes. Within this method the electronic dipersion of a nanotube is calculated from that of the corresponding 2D sheet (e.g. graphene). In this talk the problem of curvature based discrepancy between direct calculations from the tubular structure and from the related 2D sheets is examined. [1] Curvature effects of boron and carbon nanotubes of different diameters and chiralities are systematically quantified using the density functional based tight-binding method. The difference between both calculation methods can also be considered as the error of the zone-folding method. For each nanotube we quantify this error by calculating the standard deviation of the band energies and the maximal relative deviation between the derived ballistic currents. Our results indicate that quantitative predictions made using the zone-folding method may have non-negligible error.

[1] Bezugly, Eckert, Kunstmann, Kemmerich, Meskine, Cuniberti; submitted

MM 45.5 Wed 17:30 H26

Ultrashort laser-pulse excitation of a (5,0) zigzag BN nanotube — •Bernd Bauerhenne, Eeuwe Zijlstra, and Martin Garcia — Theoretische Physik - Universität Kassel - Heinrich-Plett-Str. 40, 34132 Kassel, Germany

BN nanotubes are isostructual to carbon nanotubes with boron and nitrogen atoms occupying the even and odd sublattices, respectively. In this work we investigate the laser excitation of a (5,0) zigzag BN nanotube using ab initio molecular dynamics simulations. We also analyse the mechanical properties of the nanotube in the laser-excited electronic state. We obtain a Young modulus of 920 GPa in the electronic ground state and show that this value decreases with increasing laser fluence. Our molecular dynamics simulations show that three optical phonon modes are simultaneously excited. We identify these three modes as the radial breathing mode, the radial buckling mode, and the longitudinal bond stretching mode. We demonstrate that it is possible to steer these excitation of the three modes by using a femtosecond-laser pulse train.

MM 46: Invited Talk (Hauptvortrag): Roberts

Time: Wednesday 18:00–18:30 Location: H24

Invited Talk MM 46.1 Wed 18:00 H24
Brittle-ductile transitions - cracks and dislocations — •Steve Roberts — Department of Materials, University of Oxford, OX1 3PH, UK

The interactions between loaded crack tips and dislocations are fundamental in controlling fracture behaviour and the ductile-brittle transition in simple (and some more omplex) metals, ceramics and semiconductors. Crack tips emit shielding dislocations, and can attract antishielding dislocations. These dislocations can substantially modify the crack tip stress field, leading to changes in fracture behaviour that vary with temperature via changes in dislocation nucleation and mobility. There is now a considerable body of work, both experimental and modelling, addressing these phenomena; and their combination has led to a much better understanding of the basic processes. The talk will review approaches and research in this area, and consider the new challenges and possibilities that are arising as test methods move to smaller scales and as modelling methods increase in capability, so that their usable length and time scales are now converging.

MM 47: Invited Talk (Hauptvortrag): Bennewitz

Time: Wednesday 18:30–19:00 Location: H24

Invited Talk MM 47.1 Wed 18:30 H24
Microscopic friction mechanisms on metal surfaces — •Roland Bennewitz — INM - Leibniz-Institute for New Materials, Saarbrücken, Germany

The description of friction on metal surfaces is normally based on concepts suggested by Bowden and Tabor. They identified the real area of contact, i.e. the sum of microscopic asperity contacts, as a key parameter. They also proposed how to predict contributions of shearing and ploughing to friction based on bulk properties of the materials. Friction force microscopy is an excellent tool to investigate microscopic mechanisms in friction for a single asperity. A fascinating result is the observation of a modulation of friction forces with the periodicity of the atomic surface lattice. These results are normally described by the Tomlinson-Prandtl model, a molecular ball-spring model which reflects only surface properties. We will discuss how experimental results obtained for clean metal surfaces in ultra-high vacuum challenge both descriptions. Furthermore, we will present results for the modification of microscopic friction on metal substrates by molecular lubrication layers, including graphene, self-assembled monolayers, and ionic liquids.

MM 48: Invited Talk (Hauptvortrag): Barnoush

Time: Thursday 9:30–10:00 Location: H24

Invited Talk MM 48.1 Thu 9:30 H24
Hydrogen embrittlement revisited by novel nano-mechanical approach — •Afrooz Barnoush[1,2], Mohammad Zamanzade[2], Masoud Asgari[1], Roy Johnsen[1], and Horst Vehoff[2] — [1]Norwegian university of science and technology, Trondheim, Norway — [2]Saarland university, Saarbruecken, Germany

Despite hydrogen embrittlement is known for more than a century a clear explanation of the governing mechanism is still missing. This is mainly due to the complexities of the experimental examination of hydrogen embrittlement. On the basis of these complexities a novel experimental approach, in situ electrochemical nanoindentation (ECNI), is developed. ECNI is capable of registering the onset of plasticity in extremely small volumes which can consider as perfect crystals in hydrogen free and charged conditions. It is shown that hydrogen reduces the required stress for the onset of plasticity due to reduction in the dislocation line energy. This reduction in dislocation line is explained by the Defactant Concept, i.e. reduction of the defect formation energy in the presence of hydrogen. The extent of the reduction in the dislocation line energy measured during nanoindentation can be successfully used to evaluate the intrinsic resistivity of the examined alloy or metal against hydrogen embrittlement. This makes ECNI a versatile technique for development of new hydrogen resistant alloys or coatings.

MM 49: Topical Session: Fundamentals of Fracture - Novel Experimental Techniques I

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

Topical Talk MM 49.1 Thu 10:15 H4
How crystals break - crack initiation and propagation, experiments and atomistic calculations — •Dov Sherman — Technion, Haifa, Israel

The fine details of the way brittle crystals break are still not well understood. Continuum elastodynamics based Freund energy-speed relationship suggests crack initiation at Griffith energy and propagation speed that ranges 0<V<CR. Massive atomistic computer calculations have been employed in the last two decades to resolve the fundamentals of crack initiation and propagation in brittle crystals. New effects were suggested which are not in accord with the continuum approach. The lack of sufficient experimental evidences for the theory and described effects prevent the final approval of both.

Our cleavage fracture experiments of silicon crystal show crack propagation at low speed with energy-speed relationship that apparently obeys Freund equation of motion. These findings, in addition to the fine details of the crack front, have yielded a new type of atomistic computer calculations that were able to ascertain the experimental results.

We will describe the past and present theories and phenomena associated with fracture in brittle crystals, present the fine details of the experimental results and the new atomistic calculations, and suggest a new paradigm for crack propagation sequence and energy consumption mechanisms not consider before.

MM 49.2 Thu 10:45 H4
Development and verification of an approach for determining fracture mechanical properties from tests on small size specimens — •Michael Mahler and Jarir Aktaa — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), 76344 Eggenstein-Leopoldshafen, Germany

In general, fracture mechanical properties will be identified on standard-sized specimens. Therefore special standard specifications are in use to determine J-R curves for ductile or fracture toughness for brittle fracture.
To determine fracture mechanical properties of sub-sized specimens an evaluation procedure based on finite element simulations of the crack propagation process will be used. The fracture process zone will be described by using a cohesive-zone-model (CZM). This surface based approach is able to describe the fracture mechanism in the ductile and

brittle regime selecting proper law for the constitutive traction separation. The first of the two parameters for the CZM will be experimentally determined by notched tensile tests to identify the cohesive stress. The second parameter will be found by fitting the force-deflection curve of experimental three point bending tests to the simulated one. The geometry of the sub-sized specimen is 27x3x4 mm^3 with side grooves. The applicability of the evaluation procedure will be verified on the ferritic martensitic steel T91. Therefore a comparison between standard- and sub-sized specimens is considered. The objective is to establish small size testing technology for the determination of fracture mechanical properties.

MM 49.3 Thu 11:00 H4

Micro Cantilever Bending Tests and Nanoindentation on NiAl Bond Coats and SX-NiAl — •Ralf Webler, Steffen Neumeier, Karsten Durst, and Mathias Göken — Lehrstuhl Allgemeine Werkstoffeigenschaften, Department Werkstoffwissenschaften, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland

Typically, turbine blades in aero engines and stationary gas turbines are coated with bond coats or environmental barrier coatings that are based on beta-NiAl. NiAl is an attractive intermetallic compound due to its high melting point and high Al content, which provides supreme oxidation resistance. A drawback, however, is that beta-NiAl is very brittle below the ductile to brittle transition temperature. The mechanical behavior of bond coats depends on their chemical composition, particularly important is the Al content of beta-NiAl based coatings. During service, these coatings are exposed to thermal cycling, their chemical composition changes and the mechanical properties accordingly. To determine the influence of chemical composition on hardness, Young's modulus and especially fracture toughness, bond coats with different Ni and Al content in the as-coated and thermally cycled state as well as SX-NiAl were investigated with nanoindentation and new small scaled methods. Micro cantilevers were cut by employing focused ion beam milling and subsequently in-situ bending tests were performed. This method allows to study fracture mechanics on a local scale of individual phases present in bulk materials. Results show an increase of Young's modulus with Al content and a higher hardness and fracture toughness is found in off-stoichiometric NiAl compared to binary NiAl. Furthermore, fracture surfaces differ significantly between high Ni and high Al containing samples which shows a clear influence of composition on the fracture behavior of NiAl.

MM 49.4 Thu 11:15 H4

Study on the fracture properties of NiAl single crystals by in-situ micro-cantilever bending experiments — •Johannes Ast, Karsten Durst, and Mathias Göken — Institute of General Material Properties (WW1) , Erlangen, Germany

In order to to study fracture mechanical properties on a small length scale and to understand the relation between micron-scale fracture toughness and the one of the bulk materials, in-situ and ex-situ micro-cantilever fracture tests were carried out on anisotropic NiAl single crystals. This material system offers two interesting fracture systems consisting of the soft <110> and the hard <100> orientation. The macroscopically determined fracture toughness for these two orientations is around 3-4 MPa$\sqrt{m}$ and 8-9 MPa$\sqrt{m}$ respectively. Beams of different sizes in the micron regime were prepared by Focused-Ion-Beam (FIB) machining. An AFM-based force measurement system mounted inside a Scanning Electron Microscope (SEM) was used for the in-situ experiments and a Nanoindenter XP was chosen for the ex-situ experiments. The experiments were evaluated by means of elastic-plastic fracture mechanics using the J-Integral and the crack tip opening displacement (CTOD). The discussion is focusing on the size of the plastic zone ahead of the crack tip where strong strain-gradients are formed and size effects in the flow stresses occur due to the small sample dimensions. TEM investigations and EBSD measurements of the fractured cantilevers provide detailed insights into the processes leading to fracture.

MM 50: Computational Materials Modelling - Defects & Interfaces I

Time: Thursday 10:15–11:30 Location: H24

MM 50.1 Thu 10:15 H24

Reconciling theory and experiment: Ab initio simulations of point defects up to the melting temperature — •Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

Experimental measurements of defect concentrations, enthalpies and entropies can be only performed at high temperatures close to the melting point. In contrast, presently employed T=0K and quasiharmonic DFT calculations are restricted to low temperatures. To bridge this gap a common approach is the extrapolation of the experimental data to T=0K assuming that the temperature dependence of the vacancy formation energy follows an Arrhenius behavior, i.e., that the defect entropy is independent on the temperature.

Using a newly developed approach we have been able to compute fully ab initio the temperature dependence of the defect formation energy from T=0K up to the melting point including all relevant free energy contributions, particularly also anharmonic contributions. Our results show a strong temperature dependence of the defect entropy resulting in a hitherto not expected strong non-Arrhenius behavior. Using the explicit temperature dependence we show that the T=0K extrapolated values reported in the literature are of by a few tenths of an eV for the formation energies and by an order of magnitude in the entropy. It will be shown that the revised energetics have severe consequences when using vacancy energies e.g. as benchmark to design new DFT xc functionals.

MM 50.2 Thu 10:30 H24

Stability and Mobility of Point Defects in Silicon Studied with Hybrid Density-Functional Theory Including van der Waals Interactions — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

The intrinsic point defects often significantly affect the electronic and optical properties of semiconductors; therefore their study is important from both fundamental and technological points of view. However, our understanding of self-diffusion in Si remains incomplete and full of controversies, despite decades of seminal work on the subject. Here we present a study of the stability and mobility of point defects in Si and heavier semiconductors using hybrid density-functional theory including screened long-range van der Waals (vdW) interactions [1,2]. The reduction in crystal symmetry around defect sites results in pronounced polarization, which strongly depends on the effective dimensionality of the defect. Furthermore, the screened vdW interactions promote the diffusion of interstitials by decreasing the activation energy by as much as 0.5 eV and suppress the formation of vacancies, supporting the self-diffusion mechanism proposed from P mobility experiments [3]. Notably, our calculations explain a series of experimental observations for the diffusion of interstitials, vacancies, and foreign atoms in Si. For heavier and more polarizable semiconductors, such as Ge, GaAs, and InAs, vdW interactions are found to play an increasingly important role on the stability of point defects, increasing the formation energy by as much as 0.27 eV (11.2%). [1] G. X. Zhang, *et al.*, PRL (2011). [2] A. Tkatchenko, *et al.*, PRL (2012). [3] A. Ural, *et al.*, PRL (1999).

MM 50.3 Thu 10:45 H24

Effect of exchange-correlation functionals on vacancy formation energies — •Roman Nazarov, Tilmann Hickel, and Joerg Neugebauer — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany

The key quantity that determines vacancy concentration is the vacancy formation energy. Even small uncertainties in the vacancy formation energy lead to a deviation of the vacancy concentration by several orders of magnitude. In order to analyze the performance of various exchange-correlation functionals (LDA, PBE, PW91, and AM05) in density functional theory, we calculated vacancy formation energies for 12 fcc metals [1]. The obtained results show that generally the calculated vacancy formation energies are lower than the experimental ones. Furthermore, LDA based values are systematically higher, while the PW91 are systematically lower than the PBE vacancy formation energies. A careful analysis of the possible reasons for such results shows that discrepancies between the theoretical result and experiment as

well as differences between theoretical values are mainly related to the way the various exchange-correlation functionals describe the internal surface of the vacancy. Based on this insight we propose an improved correction scheme which when postprocessing the DFT results yields a perfect alignment of vacancy formation energies for all exchange-correlation functionals. These corrected values are also in very good agreement with the experimental vacancy formation energies.

[1] R. Nazarov, T. Hickel, and J. Neugebauer, Phys. Rev. B 85, 144118 (2012)

MM 50.4 Thu 11:00 H24

Atomistic modelling of interfaces between cubic and TCP phases in FeCr — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Stainless steels show a high resistance to corrosion and radiation damage. Those effects are achieved by alloying the steel with high amounts of chromium. At elevated temperatures, however, the formation of topologically close-packed phases, in particular the σ phase is observed in FeCr systems. This σ phase is unwanted, as it increases the brittleness of the material and lowers its corrosion resistance. A first step towards a better understanding of the formation of the σ phase lies in the investigation of interfaces between the bcc and σ phase in FeCr. We employ an adaptive kinetic Monte Carlo approach to study the mobility of Fe and Cr in the different phases and to analyse atomistic processes at the interface that contribute to the transformation between the two phases. These processes can be complex, involve rearrangement of groups of atoms and can be used to form the basis for the development of a kinetic model to study the formation and growth of the σ phase on extended time scales.

MM 50.5 Thu 11:15 H24

Simulation of grain boundary mobilities in Al, Cu and γ-Fe by molecular dynamics — •Felix Ulomek and Volker Mohles — Institut für Metallkunde und Metallphysik, RWTH Aachen

The grain boundary mobility is an important physical property in metals, but its experimental determination is costly. To determine this value by molecular dynamics simulations is still a problem due to various challenges, mainly unsuited molecular dynamics atomic potentials and artificial grain boundary driving forces. We evaluate how these factors influence the migration mechanism of symmetric CSL grain boundaries in Al, Cu and γ-Fe, and calculate their migration velocities. Boundary conditions are kept as similar as possible to have these materials account for different stacking fault energies, and to show its influence on the migration behavior. Further we evaluate the effect of different MD potential types of the same element on the migration behavior and the resulting grain boundary mobility. The different sources for deviatios during the simulations are put in relation.

MM 51: Nanomaterials - Nanocrystalline & Porous Materials I

Time: Thursday 10:15–11:30 Location: H25

MM 51.1 Thu 10:15 H25

Molecular dynamics simulations of free volume redistribution in metallic nanoglasses — •Omar Adjaoud and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt, Germany

Nanoglasses are formed with glassy regions separated by interfacial areas which are called glass-glass interfaces. These interfaces influence many properties of nanoglasses such as mechanical properties. The structure arrangement at the interfaces produces excess free volume. The nanoglasses properties depend on the structure and density of their interfaces. Therefore, a detailed study of the structure and density of glass-glass interfaces is required to understand nanoglasses properties.

In the present study, we have performed molecular dynamics (MD) simulations to model excess free volume and structure of glass-glass interfaces in a metallic glass (MG) Cu64Zr36 and a MG Pd80Si20 which is a representative of metal-metalloid systems. The interactions between the atoms are described by embedded atom model. The free volume was created by randomly diluting a sphere of 1 nm radius in the simulation box of 5.8x5.8x5.8 nm dimensions for different densities with respect to the bulk glass density. For each density the system was monitored in MD runs by following the density redistribution throughout the sample with time. As a second set of simulations, a cluster of four glassy spheres of 5 nm diameter were created to form a free volume between them. The evaluation of the free volume was followed by MD simulations. The results are compared to experimental observations.

MM 51.2 Thu 10:30 H25

Investigation of the grain boundarie excess free volume in nanocrystalline $Pd_{90}Au_{10}$ under plastic deformation — •Michael J. Deckarm, Jonas Heppe, Björn Lechthaler, Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

In as-prepared nanocrystalline (nc) materials, grain boundaries (gb) are usually in a local nonequilibrium configuration, reflecting the preparation history. A two-stage recovery process of as prepared nc Pd90Au10 has been found [1]: First a reduction of the excess free volume at lower temperatures followed by grain growth at higher temperatures. Thus by careful annealing the nanocrystalline specimen below the onset temperature of grain growth, it is possible to locally equilibrate the gb by reducing their excess free volume but avoiding grain growth. As a result, the change of the free volume in the gb can be deduced by density measurements. Moreover, using calorimetry we can determine the excess enthalpy resulting from plastic deformation of the equilibrated samples, so obtaining the relation between stored excess enthalpy and excess free volume. Combining the results from XRD, density and thickness measurements, we find that deformation is accompanied by reduction of excess free volume.

[1] A. Tschöpe, R. Birringer and H. Gleiter; Calorimetric Measurements of the Thermal Relaxation in Nanocrystalline Platinum; Journal of Applied Physics (USA). Vol. 71, no. 11, pp. 5391-5394. 1 June 1992

MM 51.3 Thu 10:45 H25

Stabilization of Nanocrystalline Iron by Segregation of Carbon at the Grain Boundaries — •Marie Christine Trynogga[1], Andreas Herz[2], Yuzeng Chen[3], Christine Borchers[1], and Reiner Kirchheim[1] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]TU Ilmenau, FG Werkstoffe und Elektrotechnik, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau — [3]State Key Lab of Solidification Processing, Northwestern Polytechinical Univeristy, Xi'an, China

A nanocrystalline iron-carbon alloy was produced by high-energy ball milling to experimentally confirm the *defactants* (**def**ect **act**ing **agents**) concept, which was introduced in [1]. For this system the *defactants* concept predicts that the carbon atoms act as segregating solute atoms, i.e. the carbon is enriched at the grain boundaries and significantly reduces the grain boundary energy. So the formation of grain boundaries is favoured, stabilizing the grain boundaries leading to a nanocrystalline structure.

Iron powder was mixed with graphite reaching carbon concentrations of up to 4.3 wt.%. The samples were produced by high-energy ball milling. The microstructure was investigated by X-ray diffraction (XRD) and transmission electron microscopy (TEM). It was observed that the α-iron structure persists and the grain size decreases with increasing carbon concentration. This dependence follows from the *defactants* concept connected with a simple mass balance of carbon in a closed system.

[1] R. Kirchheim, Acta Materialia 55 (2007) 5129 and 5139

MM 51.4 Thu 11:00 H25

Solid solution strengthening in nanocrystalline Pd-Au alloys — •Andreas Leibner[1], Manuel Grewer[1], Christian Braun[1], Jonas Heppe[1], Jochen Lohmiller[2], Patric Gruber[2], and Rainer Birringer[1] — [1]Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2 2, 66123 Saarbrücken — [2]Karlsruher Institut für Technologie, Institut für Angewandte Materialien, Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen

It is well known that nanocrystalline (nc) materials show enhanced mechanical properties depending on their grain size. In binary al-

loys, solute drag enhances the stability of the nanoscale microstructure. However, systematic studies on the influence of solute content on the mechanical response of nc alloys with constant grain size are still scarce. Here we report on the influence of gold concentration on the strength of nc Pd-Au with 10nm-sized grains. The samples were prepared by inert gas condensation and tested in shear-compression-specimen (SCS) geometry. While all Pd-Au compositions show the typically increased strength due to grain refinement, the overall trend is a fairly linear strength decrease with rising gold concentration. In contrast, Vickers hardness measurements on arc melted coarse grained Pd-Au alloys exhibit classical solid solution hardening.

MM 51.5 Thu 11:15 H25

Following the deformation processes of nanocrystalline PdxAu1-x by the combination of in-situ straining and ACOM-TEM — •Aaron Kobler[1,2], Christian Kübel[1], and Horst Hahn[1,2] — [1]Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany — [2]Technische Universität Darmstadt (TUD), 64287 Darmstadt, Germany

Understanding the deformation mechanisms in nanocrystalline (nc) metals and alloys is crucial for improving their performance and stability as needed for technical applications. Most of our current understanding stems from in-situ deformation experiments on bulk nc materials using XRD. However, it is difficult to understand the local processes based on bulk measurements. The local processes are traditionally investigated using classical BF/DF-TEM. Recently, ACOM-TEM is used instead of BF/DF-TEM as it identifies the crystallographic orientation of all crystallites and detects all CSL special boundaries within the imaged area. We have implemented the ACOM-TEM (NanoMegas) on a FEI Tecnai-F20 in micro-probe (up) STEM mode, that allows us to acquire (fast) STEM reference images. We combined ACOM-TEM imaging with in-situ straining inside the TEM using Hysitron's TEM Picoindenter using steps of increasing strain. First investigations were conducted on magnetron sputtered Au samples. Deformation of this film inside the TEM allowed us to follow the continuous process of grain growth and grain rotation in nc Au with increasing strain. New results on the influence of alloying content in PdxAu1-x on the deformation mechanisms will be discussed.

MM 52: Phase Transformations I

Time: Thursday 10:15–11:30 Location: H26

MM 52.1 Thu 10:15 H26

MELTING AND STRUCTURAL BEHAVIOUR OF INDIUM NANOPARTICLES EMBEDDED IN AN ALUMINIUM MATRIX — •Mostafa Mohamed, Martin Peterlechner, Tae Eun Song, and Gerhard Wilde — Institute of Materials Physics,Münster,Germany

The melting behaviour of small crystalline solid particles has attracted the interest of many researchers. In the present work, an alloy of Al-4 at % In with nanoparticles of Indium embedded in an Aluminium matrix was synthesized by rapid quenching using the melt-spinning technique. The melting point and freezing behaviour of the embedded nanoparticles were investigated using differential scanning calorimetry and transmission electron microscopy (TEM) including high resolution transmission electron microscopy (HRTEM). DSC experiments showed broad melting and crystallization peaks. The crystallization temperature of the embedded particles shifted to remarkable low temperature. The microstructure exhibited a homogeneous distribution of facetted In particles embedded in the Al-matrix. Analyses of HRTEM images were done to analyse the topology of the heterophase interfaces between Al and In in detail. The results are discussed with respect of the impact of the mismatch accommodation of interfaces on the thermodynamics of nanoscale systems.

MM 52.2 Thu 10:30 H26

Analysis of the melting point depression and the structure of Bi nanoparticles embedded in Zn matrix — •Tae-Eun Song, Martin Peterlechner, and Gerhard Wilde — Institute für Materialphysik, Wilhelm-klemm-straße 10, D-48149 Münster, Germany

The melting point depression of embedded Bi nanoparticles in a Zn matrix synthesized by rapid solidification was analyzed using Differential Scanning Calorimetry (DSC) and Transmission Electron Microscopy (TEM). TEM shows an elongated and faceted morphology of Bi nanoparticles. The elongated Bi particle (012) facet is arranged parallel to Zn (002). Upon heating in the DSC two Bi melting signals occur, one close to the bulk melting temperature and the other at a lower temperature. Subsequent cooling leads to two solidification signals. During repeated heating and cooling, some Bi particles are solidified at a small undercooling with a number of exothermic peaks, whereas other Bi particles are solidified with a broad exothermic peak at a larger undercooling. Thermal cycling below the bulk Bi melting temperature leads to a gradual decrease of the solidification enthalpy at larger undercoolings. The results are discussed in the framework of size confinement and interface control of phase transformations.

MM 52.3 Thu 10:45 H26

Investigation of solidification dynamics of Zr-based alloys — •Raphael Kobold[1,2] and Dieter Herlach[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany

In contrast to experiments with most undercooled binary alloys the velocity of dendritic growth of a Cu50Zr50 alloy does not increase monotonically with undercooling but passes through a maximum and then decreases. To study this behaviour we investigate Zr-based alloys such as CuZr, NiZr and NiZrAl with Zirconium concentrations ranging from 36 to 64 at.% including eutectic and intermetallic phases. We use electrostatic levitation technique to melt and undercool samples with a diameter of 2-3 mm under ultra-high-vacuum conditions. Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures since heterogeneous nucleation on container walls is completely avoided. During crystallisation of the undercooled melt the heat of crystallisation is released. The rapid increase of the temperature at the solid-liquid interface makes the solidification front visible. The velocities of the solidification front are recorded by using a high-speed camera with a maximum rate of 50.000 frames per second and are analyzed with a software for optical ray tracing. Furthermore, we try to model the growth velocity vs. the undercooling temperature and perform sample EBSD analysis with a scanning electron microscope. This project is funded by Deutsche Forschungsgemeinschaft, under grant HE1601/26-1.

MM 52.4 Thu 11:00 H26

investigation of nucleation in undercooled melts of pure Ni and Co100-xPdx alloy — •Reeti Singh[1,2], Gerhard Wilde[3], and Dieter Herlach[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Institut für Materialphysik, Westfaälische Wilhelms-Universität Münster, 48149 Münster, Germany

Nucleation initiates the formation of a new phase within the environment of the parent phase. It is the phenomenon in nature and technology which is involved in a large variety of phase transformation. In the present work nucleation in undercooled pure Ni and Co80Pd20 is investigated. Levitation and calorimetry techniques were applied to undercooled melts of pure Ni and Co80Pd20. Each sample was undercooled several times (˜ 80-100 cycles) and the distribution function of undercooling is determined. The evaluation of the undercooling distribution function in the frame work of the Skripov model yields information about the free energy barrier and the pre-exponential factor to distinguish between heterogeneous and homogeneous nucleation. The free energy barrier and pre-exponential factor was extracted from the measured nucleation rates obtained by using histogram method. The expected value of free energy barrier and pre-exponential factor for homogenous nucleation in case of pure Ni and Co80Pd20 are 74 kBT and 1039 m-3s-1 respectively.

MM 52.5 Thu 11:15 H26

Measurement of nucleation rates using fast scanning calorimetry on samples prepared by the Droplet Emulsion Technique (DET) — •Christian Simon, Joachim Bokeloh, and Gerhard Wilde — Westfälische Wilhelms-Universität, Institut für

Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The most difficult part in experiments on heterogeneous nucleation is the control of the heterogeneous nucleant. On one hand, parasitic nucleants like the container wall and impurities must be removed, and on the other hand the target nucleant phase must be kept at a constant potency. The DET is used to reduce the influence of impurities by dispersing a bulk volume to a fine dispersion of droplets. During the emulsification, a low-catalytic surface coating is applied to reduce the nucleation potency of the surface. The nucleation rate is evaluated by a statistical analysis that treats nucleation as a non-homogenous Poisson process and leads to model-free values of the nucleation rate. A fast scanning nano-calorimeter (10 K/s - 10000 K/s) is used to analyze the nucleation rate over a large number of repeated heating-cooling-cycles on a single droplet. We present experimental data on tin and a tin-bismuth alloy, which were both prepared by DET. Large values of undercooling were observed in tin. Indications of the formation of a metastable phase at large undercooling were observed in the tin-bismuth alloy. In additional experiments, the Sn-Bi alloys were only partially melted and the residual crystalline phase was used to act as heterogeneous nucleation-site.

MM 53: Topical Session: Fundamentals of Fracture - Novel Experimental Techniques II

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

MM 53.1 Thu 11:45 H4

Investigation of the fracture behavior of Tungsten at the micro scale — •Nicola Julia Schmitt[1], Christoph Bohnert[1,2], Christoph Eberl[1], Oliver Kraft[1], and Sabine Maria Weygand[2] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen (Germany) — [2]Department of Mechanical Engineering and Mechatronics, Karlsruhe University of Applied Sciences, 76133 Karlsruhe (Germany)

Tungsten promises great potential as structural material in power generation due to its high melting point. One challenge however, is to deal with its ductile-to-brittle transition far above room temperature which limits its application. Studies at the macro scale have shown that microstructural characteristics have a big influence on the fracture toughness of tungsten. Moreover, it was shown that tungsten can be fairly ductile at small scale for sample sizes below 100 μm. To deepen the insight into the underlying fracture mechanisms, tests are carried out at the micro scale, which are supported by finite element simulations.

To investigate the influence of the crystal orientation and grain boundaries two different types of beams were tested, namely single crystal microbeams with different orientations and bi-crystalline microbeams with varied grain boundary orientations. The micro bending beams with 30 μm in width and 200 μm in length have been fabricated and notched by a combined method of micro-electro-discharging machining and focused ion beam. Fracture experiments are conducted by using a nanoindentation system. First results indicate that fracture is rather brittle when the notch is aligned an expected cleavage plane.

MM 53.2 Thu 12:00 H4

Cracking in 'nanocomposite' CrAlN/Si3N4 hard coatings — Shiyu Liu[1], Jeff Wheeler[2], Philip R. Howie[1], Xiangting Zeng[3], Johann Michler[2], and •William J. Clegg[1] — [1]Gordon Laboratory, Department of Materials Science & Metallurgy, Pembroke St, Cambridge CB2 3QZ, UK — [2]EMPA, Feuerwekerstrasse 39, CH-3062 Thun, CH — [3]Singapore Institute of Manufacturing Technology, 71 Nanyang Drive, Singapore 638075

Recent work has shown that the flow behaviour of hard coatings of a very fine-grained CrAlN/Si3N4 is similar to that predicted by expanding cavity type models. However, preliminary observations suggest that the cracking behaviour of these materials is somewhat different to that observed in more conventional CrAlN hard coatings. In this paper, a double cantilever beam method has been developed to study the nature of crack growth in hard coatings. The test method is first described, including a way of correcting for frictional effects between the punch and the sample. The measured values of the crack resistance of SiC and GaAs are compared with those obtained at larger scales. The method is then used to measure the resistance to cracking in different hard CrAlN-based coatings and to study how a crack grows through the coating and the influence of the coating microstructure.

MM 53.3 Thu 12:15 H4

Bulge testing as a tool for investigating the fracture properties of thin films - Application to silicon nitride and gold membranes — •Benoit Merle and Mathias Göken — Department of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, Germany

The bulge test was developed into a valuable tool for investigating the fracture mechanism of very thin films (30 - 300 nm). The improved sample preparation includes milling a crack-like slit in the center of the membrane, using a Focused Ion Beam. The samples are then pressurized in the bulge test until failure occurs. Optionally, the experimental setup is inserted into an AFM, which allows in-situ imaging of the extension of the crack. The presentation will show applications on thin amorphous silicon nitride and nanocrystalline gold films. As a brittle material, silicon nitride is well suited for the quantitative measurement of the fracture toughness KIC. The bulge test results show that the fracture toughness does not depend on the thickness of the SiNx film, although its state changes from plane-strain to plane-stress. Since gold is a more ductile material, the focus was laid on the in-situ AFM observations of the crack propagation. Grain boundary sliding was observed to occur in these thin films, which probably accounts for the low toughness found for gold thin films.

MM 53.4 Thu 12:30 H4

The Effect of Prior Heat Treatment on the Fracture Energy of Metal Fibre Reinforced Ceramic Composites (MFCs) — •Su Ki Lam, Louise Gale, and Bill Clyne — Department of Materials, Pembroke Street, Cambridge CB2 3QZ UK

This work concerns the fracture energy of alumina matrix composites with (˜15vol%) steel fibres. A recent model [1] gives the work of fracture from pull-out and/or plastic deformation of fibres bridging the crack plane. The present work concerns exposure to high temperature (˜1,000C). The standard fibre is 304, with strength and ductility that confer toughness on the composite, mainly from fibre plasticity. However, this steel has poor oxidation resistance. Since the matrix offers little environmental protection, this oxidation can be extensive, reducing ductility and creating defects within the composite. The toughness can thus fall sharply after heat treatment. The study also covers another steel (310) with superior oxidation resistance. Fibres of 310 exhibit lower strength and ductility than 304 (as-received), but are less prone to oxidation-induced degradation of these properties. The fracture energy after heat treatment can thus be higher with 310 fibre, and fracture energy values are consistent with model predictions and experimental single fibre tensile data. Results are also presented concerning oxidation and microstructural changes. [1] S.R. Pemberton, E.K. Oberg, J. Dean, D. Tsarouchas, A.E. Markaki, L. Marston & T.W. Clyne, The fracture energy of metal fibre reinforced ceramic composites (MFCs), Composites Science and Technology, vol.71 (2011) p.266-275.

MM 53.5 Thu 12:45 H4

Plasticity and fracture in drying colloidal films — •Lucas Goehring[1], William J. Clegg[2], and Alexander F. Routh[3,4] — [1]MPI Dynamics and Self-Organization, Göttingen, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, UK — [3]Department of Chemical Engineering and Biotechnology, University of Cambridge, UK — [4]BP Institute for Multiphase Flow, University of Cambridge, UK

Cracks in drying colloidal dispersions are typically modelled by elastic fracture mechanics, which assumes that all strains are linear, elastic, and reversible. We tested this assumption in films of a hard latex, by intermittently blocking evaporation over a drying film, thereby relieving the film stress. Here we show that although the deformation around a crack tip has some features of brittle fracture, only 20-30% of the crack opening is relieved when it is unloaded. Atomic force micrographs of crack tips also show evidence of plastic deformation, such as micro-cracks and particle rearrangement. Finally, we present a simple scaling argument showing that the yield stress of a drying colloidal

film is generally comparable to its maximum capillary pressure, and thus that the plastic strain around a crack will normally be significant. This also suggests that a film's fracture toughness may be increased by decreasing the inter-particle adhesion.

MM 54: Computational Materials Modelling - Defects & Interfaces II

Time: Thursday 11:45–13:00 Location: H24

MM 54.1 Thu 11:45 H24

Neural Network Studies of the Interface between Copper and Zinc Oxide — •Björn Hiller, Nongnuch Artrith, and Jörg Behler — Lehrstuhl für Theoretische Chemie Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Despite its importance as a catalyst in e.g. the methanol synthesis, the atomistic structure of copper clusters supported at zinc oxide is not fully understood. It was experimentally shown that copper entrenches into the zinc oxide upon heating. This indicates strong interactions between the copper particles and the underlying support, whose origins and implications are not resolved up to now. Theoretical studies of such systems is demanding due to the inherent problem of the lattice mismatch between the subsystems. Using standard DFT calculations one is currently limited to a few hundred atoms which only allows to investigate rather small interfaces. In the present work we explore the applicability of more efficient Neural Network potentials to describe the structural and energetic properties of a variety of copper-zinc oxide interface models.

MM 54.2 Thu 12:00 H24

Ab initio stacking fault energy calculations in Mg-Y alloys — •Zongrui Pei[1,2], Stefanie Sandloebes[1], Stefan Zaefferer[1], Alexey Dick[1], Martin Friak[1], Li-Fang Zhu[1], Sangbong Yi[3], Dietmar Letzig[3], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]2Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — [3]Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Geesthacht, Germany

Pure magnesium and most commercial wrought magnesium alloys exhibit a low room temperature ductility which can be significantly increased by the addition of Y or rare earth elements (Acta Mater. 59 (2011) 429). Under- standing the mechanisms causing this ductility enhancement on an atomistic and electronic-structure level would provide a systematic approach to identify alternative favorable solutes. Therefore, in order to obtain a deeper insight into the mechanisms active in the Mg-Y alloys, a quantum-mechanical (so called ab initio) study of the compositional dependence of intrinsic stacking fault (ISF) energies has been performed. Employing density functional theory (DFT) calculations, the ISF energies have been determined within the Axial Next-Nearest-Neighbour Ising (ANNNI) model. An in-depth analysis of the theoretical data shows reduced ISF energies as a direct consequence of the dramatically reduced thermodynamic stability of hexagonal Mg-Y solid solutions when the Y concentration approaches its solubility limit in Mg (Acta Mater. 60 (2012) 3011).

MM 54.3 Thu 12:15 H24

Ab initio and atomistic study of generalized stacking fault energies in Mg and Mg-Y alloys — •Li-Fang Zhu[1], Zongrui Pei[1,2], Stefanie Sandloebes[1], Johann Pezold[1], Martin Friak[1,2], Stefan Zaefferer[1], Howard Sheng[3], Chris Race[1], Bob Svendsen[1,2,4], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — [3]George Mason University, Fairfax, USA — [4]Faculty of Georesources and Materias Engineering, RWTH Aachen, Aachen, Germany

Mg-Y alloys show significantly improved room temperature ductility when compared with pure Mg. We study this interesting phenomenon theoretically at the atomic scale employing quantum-mechanical and atomistic modeling methods. Specifically, we have calculated generalized stacking fault energies for five slip systems in both elemental magnesium (Mg) and Mg-Y alloys using (i) density functional theory (DFT) and (ii) a newly developed embedded-atom method (EAM) Mg-Y potential. These calculations predict that the addition of Y results in a reduction in the unstable stacking fault energy of basal slip systems. In case of I_2 stacking fault, the predicted reduction of the stacking fault energy due to Y atoms was verified by experimental TEM measurements. We find a similar reduction for the stable stacking fault energy of the 11-22<11-23> non-basal slip system. On the other hand, other energies along this particular γ-surface profile increase with the addition of Y.

MM 54.4 Thu 12:30 H24

Surface chemistry in a full-potential QM/MM approach: making hybrids affordable — •Daniel Berger[1], Volker Blum[2], and Karsten Reuter[1] — [1]TU München — [2]Fritz-Haber Institut der MPG

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. When addressing corresponding functionalities through quantitative first-principles calculations, exploitation of the localized character of the chemical processes yields numerically most efficient approaches. To this end we augment the FHI-aims [1] package with a QM/MM [2] functionality, in which the nanostructure and immediate oxide surrounding is described quantum mechanically, the long-range electrostatic interactions with the support are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the accuracy and efficiency of the implementation with examples from the photo-catalytic water splitting context and specifically discuss the use of charged system states to address charge transfer processes.

[1] V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175 (2009)
[2] N. Bernstein *et al.*, Rep. Prog. Phys., **72**, 026501 (2009)

MM 54.5 Thu 12:45 H24

Reliable Modeling of Complex Organic/Metal Interfaces — •Wei Liu, Sergey Filimonov, Victor G. Ruiz, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

The understanding of electronic properties of complex organic/metal interfaces requires a reliable method for the prediction of their structure and stability. The bonding at complex interfaces arises from delicate balance between covalent bonds, van der Waals (vdW) forces, charge transfer, and Pauli repulsion. Recently, we developed a method based on density-functional theory with vdW interactions (PBE+vdW^{surf} [1]) to accurately model adsorbates on surfaces, by a synergetic linkage of the PBE+vdW method [2] for intermolecular interactions with the Lifshitz-Zaremba-Kohn theory [3] for the dielectric screening within the substrate surface. This method is demonstrated to reliably model a multitude of small and large molecules on metal surfaces [1,4,5], leading to an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies with respect to state-of-the-art experiments. To demonstrate the predictive power of the PBE+vdW^{surf} method, we design a novel type of single-molecule push button switch, by carefully controlling the stability and activation barrier between a chemically bound state and a physically bound state for benzene derivatives adsorbed on metal surfaces.

[1] Ruiz, *et al.*, PRL (2012). [2] Tkatchenko and Scheffler, PRL (2009). [3] Zaremba and Kohn, PRB (1976). [4] Al-Saidi, *et al.*, Nano. Lett. (2012). [5] Wagner, *et al.*, PRL (2012).

MM 55: Nanomaterials - Nanocrystalline & Porous Materials II

Time: Thursday 11:45–13:00 Location: H25

MM 55.1 Thu 11:45 H25

Structural and thermodynamic properties of severely deformed nickel — •Daria Prokoshkina[1], Anna Moros[1], Vladimir Popov[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Institute of Physics of Metals, Russian Academy of Science, Ekaterinburg, Russia

The effect of severe plastic deformation (SPD) on microstructure, thermodynamic and transport properties of Ni of 99.6 wt. % purity was investigated. The plastic deformation was realized via equal channel angular pressing (ECAP), high-pressure torsion (HPT) and by cold rolling (CR) to 80 %. The properties of ultrafine grained nickel prepared by room temperature deformation (ECAP, HPT, CR), warm deformation at 200°C (ECAP), and cold deformation at liquid nitrogen temperature (HPT) were compared. The influence of different deformation paths on the microstructure was studied by Scanning Electron Microscopy with Focused Ion Beam add-on. Differential Scanning Calorimetry was used to analyze the thermally induced defect recovery. Grain boundary diffusion measurements were used to characterize the kinetic properties of interfaces in deformed and annealed materials applying the radiotracer technique and the 63Ni radioisotope. The obtained results are discussed concerning the impact of the deformation pathway on the kinetic and microstructural properties.

Financial supports of German-Israel Foundation (GIF) through research Grant No: G-1037, Deutscher Forschungsgemeinschaft and Russian Foundation for Basic Research (grant No: 12-03-91331-NNIO) are acknowledged.

MM 55.2 Thu 12:00 H25

Molecular dynamics study of nanoporous gold deformation — •Bao-Nam D. Ngo[1,2], Karsten Albe[2], and Jörg Weissmüller[1,3] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

Nanoporous gold made by dealloying is under discussion for applications in actuation, catalysis, and sensing. The material is also a model system for deformation processes in nanomaterials. While early experiments suggest that nanoporous gold is brittle, recent studies reveal its ductile behavior in compression test, with many striking observations, such as a yield strength lower than what is expected from scaling law, nearly zero transverse plastic flow, and extremely high strain hardening coefficients. Here, we report a molecular dynamics study of the deformation of nanoporous gold, focused on uniaxial compression tests. Computer samples are prepared by spinodal decomposition. In agreement with experiment, they show ductile behavior with low yield stress, very small transverse plastic strain, and an extended elastic-plastic transition region in the stress-strain curve. The underlying deformation mechanisms and dislocation activity are investigated.

MM 55.3 Thu 12:15 H25

Elastic and plastic behavior of nanoporous gold as a function of the surface state — •Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, 21502 Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, 21073 Hamburg, Germany

Nanoporous metal is a bicontinuous network of nanoligaments interpenetrated by an open pore space. It exhibits an extremely high specific surface area, which is accessible to electric signals, that afford the surface properties tuning. In this way, the macroscopic materials behavior can be reversibly modified. Here, we report an *in situ* study on mechanical properties of bulk nanoporous gold infiltrated with electrolyte. The metal-liquid interface properties were controlled via the electrode potential, E. This allowed reversible variations between 1) adsorbate-covered and bare or 2) electrically charged and charge-neutral surface states. The environmental control was implemented in a dynamic mechanical analyzer (DMA) and mechanical testing machine, and revealed large reversible cyclic changes of the effective elastic modulus and flow stress. The results advertize a role of two higher derivatives of the surface free energy function $\psi(E, e)$ where e denotes the strain. The parameter $\mathrm{d}^2\psi/\mathrm{d}e^2$ represents an excess elastic constant of the surface. The potential dependence of this behavior, probed in our DMA experiments, relates to the third derivative, $\mathrm{d}^3\psi/(\mathrm{d}e^2\mathrm{d}E)$. Our data present first evidence for this quantity and support the notion of tuning the elasticity and plasticity via the applied electric potential.

MM 55.4 Thu 12:30 H25

Synthesis of nanoporous gold for electrochemical actuators — •Yi Zhong[1], Jürgen Markmann[1,2], Hai-Jun Jin[3], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [2]Institut für Werkstoffphysik und Technologie, Technische Universität Hamburg-Harburg, Hamburg, Germany — [3]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, P.R. China

Dealloying, an alloy corrosion process of gold alloys was used to fabricate nanoporous gold (npg) with a porosity up to 80 % and structural sizes, i.e. ligament diameters, down to a few nanometers. Particularly, the formation of macroscopic cracks has been investigated for two different starting alloy compositions, Au25Ag75 and Au25Cu75 which represent substitutional solid solutions with more or less identical atom size (Au-Ag) and very different atom size (Au-Cu). Apart from the dealloying potential, different pretreatments of the starting consequently provided completely different microstructural starting conditions and were compared with respect to their ability to suppress cracks in the resulting nanoporous structure. The resulting samples were crack-free with ligament sizes below 10 nm. Within different electrolyte environments, the amplitude of actuation of this npg could be tuned to values up to 0.89 %. Npg with such small ligament sizes are expected for application in electrochemical actuators of high functionality.

MM 55.5 Thu 12:45 H25

Diffusion-induced recrystallization in Si/Ge — •Michael Kasprzak, Sebastian Manuel Eich, Dietmar Baither und Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität, Münster

In size-mismatched thin film interdiffusion couples, Diffusion-Induced Recrystallization (DIR) appears rather than conventional Fickian interdiffusion. New grains formed in the diffusion zone reveal characteristic stepwise composition levels. Based on experiments with metallic thin films, we derived recently a quantitative model which combines thermo-elastic driving forces and grain boundary migration [1-3]. Observed concentration levels are such that the stress in front of the moving grain boundary reaches a maximum. This stress is rather high, close to the theoretical maximum strength of the material at the relevant temperature. In new experiments, we study this effect in semiconductor layers, Ge on Si, for the first time. Heat treatment was performed in two stages: first annealing at 650°C to crystallize the pure Ge layer; second annealing at higher temperatures to initiate interdiffusion. Transmission electron microscopy and energy dispersive X-ray spectroscopy show that new grains of characteristic composition are indeed formed towards the Ge side of the diffusion couple similar as previously observed with fcc metals. Characteristic concentrations are derived from XRD data and compared with the suggested model.

[1] Schmitz et al. Scr Mater 63 (2010) 484; [2] Kasprzak et al. Acta Mater 59 (2011) 1734; [3] Eich et al. Acta Mater 60 (2012) 3469

MM 56: Phase Transformations II

Time: Thursday 11:45–13:00 Location: H26

MM 56.1 Thu 11:45 H26

Dendrite growth kinetics of undercooled Iron-based alloy melts — •Christian Karrasch[1,2], Thomas Volkmann[1], and Dieter M. Herlach[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany

Dendritic growth is the major crystal growth mode controlling the evolution of the microstructure during solidification of metallic alloys. In order to verify models for dendritic growth in undercooled melts growth velocities were measured on pure Fe and Fe-based alloy melts. We analyse the effect of solute redistribution on the growth of Fe-B revealing a small partitioning coefficient. Electromagnetic levitation technique is applied to undercool droplets of metallic melt accessible for in-situ diagnostics of the solidification processes. Deep undercoolings of more than 200 K prior to solidification are achieved, which leads to rapid growth of dendrites with velocities of several m/s. The temperature-time profile is measured by a pyrometer while rapid solidification is monitored by a high-speed video camera. The contrast between the liquid and solid phase is visible due to the release of latent heat during recalescence. Experimental results will be presented and discussed in the frame of current model for dendritic growth in undercooled melts.

This research work is supported by the German Research Foundation DFG within contract HE1601/18 and ESA within the project CCEMLCC under contract no. 4200020277.

MM 56.2 Thu 12:00 H26

Simulation of rapid crystallization in phase change materials by means of phase field modeling — •Fatemeh Tabatabaei[1], Markus Apel[2], and Efim Brener[1] — [1]Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, 52428 Jülich — [2]Access e.V., RWTH Aachen, 52072 Aachen

Phase change materials (PCM) are employed in data-storage applications extensively. A stable crystalline and a metastable amorphous state can be utilized for the data recording. To obtain a quantitative understanding of the kinetics of writing and erasing data, it is essential to gain insights into the energy transport and phase boundary movement during the phase transformation. We applied phase field modeling as a continuum simulation technique in order to study rapid crystallization processes in AgInSbTe. The simulation model is adapted to the experimental conditions, in particular the geometrical arrangement used for measurements of crystallization rates by a laser pulse technique. Simulations are performed for substrate temperatures close to the melting temperature of AgInSbTe down to low temperatures when an amorphous state is involved. Different growth regimes are identified by calculating crystallization velocity as a function of undercooling. We discussed the role of interface mobility on solidification kinetics by determining the mobility as a function of temperature. Furthermore, the role of nucleation of the crystalline phase as well as temperature dependent thermophysical properties are investigated.

MM 56.3 Thu 12:15 H26

Spinodal decomposition versus nucleation and growth mechanism of phase separation in nonstoichiometric silicon oxide films during high temperature annealing — •Andrey Sarikov — V. Lashkarev Institute of Semiconductor Physics NAS Ukraine, 45 Nauki avenue, 03028 Kiev, Ukraine

This work is devoted to the study of the thermodynamic mechanisms of phase separation in the nonstoichiometric silicon oxide films during high temperature anneals. Based on the obtained earlier expression for the Gibbs free energy of nonstoichiometric silicon oxide phase, the binodal and the spinodal characteristics of silicon oxide as well as the regions of stoichiometry indexes corresponding to the stability, metastability, and instability of silicon oxide phase with respect to the phase separation as the functions of temperature are determined. The regions of the phase separation process taking place according to the spinodal decomposition and according to the nucleation and growth mechanism are presented. Obtained results are useful for the development of the kinetic theory of phase separation in nonstoichiometric silicon oxide films and the formation of the structures consisting of Si nanoinclusions in the silicon oxide matrix.

MM 56.4 Thu 12:30 H26

Experimental examination of the MacPherson-Srolovitz prediction for grain growth kinetics — •Jules Dake[1], Jette Oddershede[2], Søren Schmidt[2], and Carl Krill[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Department of Physics, Technical University of Denmark, Denmark

The long-sought extension of the von Neumann relation to 3D — recently achieved by MacPherson and Srolovitz — constitutes a major advance in the field of materials modeling. If, however, this new relation is to serve as the basis for predicting microstructural evolution, then it must be tested against real three-dimensional coarsening data, which has proven stubbornly difficult to come by. Fortunately, the recently developed technique of three-dimensional x-ray diffraction microscopy (3DXRD) has made it possible to map the 3D microstructure of a polycrystalline sample nondestructively, delivering exactly the kind of experimental data required to test the MacPherson-Srolovitz relation. In a previous attempt, the authors successfully mapped and characterized a polycrystalline Al-1wt.% Mg specimen before and after heat treatment at 350°C. Regrettably, the annealing step (90 min) was too long, rendering an analysis of the local growth kinetics impossible. This time, we repeated the experimental procedure using intervals just 10 min in duration, and we extracted the local growth kinetics from a total of 9 time steps. The measured growth rates of individual grains are finally compared to predictions of the MacPherson-Srolovitz relation.

MM 56.5 Thu 12:45 H26

Impact of the inclination dependence of grain boundary energy on faceting and kinetics of grain boundaries in Aluminum — •Jann-Erik Brandenburg, Dmitri A. Molodov, and Luis A. Barrales-Mora — Institute of Physical Metallurgy and Metal Physics, RWTH-Aachen University

The motion and faceting behaviour of <100> tilt and mixed tilt-twist grain boundaries with misorientations in the range between 4° and 23° were investigated in situ in a scanning electron microscope at elevated temperatures. The results revealed that tilt boundaries with misorientations lower than 15° did not assume a curved shape and did not move under a capillary driving force at any temperature. In contrast, all investigated low angle boundaries with mixed tilt-twist geometry (20° twist component) were observed to attain a smoothly curved shape and moved under a curvature force. Molecular static simulations provided evidence that the experimentally observed behaviour is due to the inclination dependence of grain boundary energy, which is very pronounced for pure tilt (low angle) boundaries but becomes nearly isotropic for mixed boundaries with the same rotation angle. The influence of the energy anisotropy on grain boundary migration during grain growth was investigated by molecular dynamic simulations of shrinking initially circular grains encircled by tilt and mixed boundaries. The results showed an influence of the inclination dependent energy on the shape of the grains during shrinking as well as on the shrinking rate itself.

MM 57: Invited Talk (Hauptvortrag): Ivanisenko

Time: Thursday 15:00–15:30 Location: H24

Invited Talk MM 57.1 Thu 15:00 H24

Micro- and macroplastic behavior of nanocrystalline Pd-Ag alloy in temperature range between 4 and 300K — •Yulia Ivanisenko — Institut für Nanotechnologie, Karlsruher Instut für Technologie, 76021 Karlsruhe, Germany

Nanocrystalline (nc) materials with the mean grain size as small as 15-30 nm demonstrate very peculiar mechanical behavior, for example, strong compression/tension asymmetry, extended elastic-to-plastic transition (extended microplasticity stage), propensity to strain localization, stress-induced grain growth and abnormally high cryogenic strength. Taking nc Pd-Au alloy prepared by inert gas condensation method as example, these peculiarities were studied using various ex situ and in situ testing techniques including in situ SEM compression test, compression test in the temperature range between 4 - 300 K, instrumented high pressure torsion and synchrotron texture measurements. In this contribution, the overview of the obtained results will be given and discussed.

MM 58: Topical Session: Fundamentals of Fracture - Fatigue Fracture

Time: Thursday 15:45–17:00 Location: H4

Topical Talk MM 58.1 Thu 15:45 H4

Nucleation and interaction of cracks at and with interfaces — •Horst Vehoff — Institut für Werkstoffwissenschaft, Universität des Saarlande, Saarbrücken

Fatigue and crack growth tests on nano and macro sized bi- and polycrystals are presented. The focus of the experiments lies on the interaction of cracks with defined interfaces as well as on the effect of grain size on crack growth especially in bimodal microstructures of the nano - ufg type. Special techniques like 3D- tomography, EBSD, OGM and STEM are used to characterize the cracks. The results are discussed in the view of recent crack growth models.

MM 58.2 Thu 16:15 H4

Propagation Behaviour of Microstructurally Short Fatigue Cracks in the High Cycle and Very High Cycle Fatigue Regime — •Hans-Jürgen Christ[1] and Claus-Peter Fritzen[2] — [1]Institut für Werkstofftechnik, Universität Siegen, Germany — [2]Institut für Mechanik und Regelungstechnik - Mechatronik, Universität Siegen, Germany

It is generally accepted that crack initiation mechanisms and short fatigue crack propagation processes govern fatigue life in the high and very high cycle fatigue regimes. Local slip irreversibility causes crack initiation far below the fatigue limit. However, interaction of the crack tip with microstructural barriers, such as grain boundaries or second phases, leads to a decrease and eventually to a stop in the crack-propagation rate. If this is the case even for the weakest site the fatigue limit is reached. In the present contribution examples for propagating and non-propagating conditions of short fatigue cracks are given for a single-phase beta-titanium alloy, a duplex steel, a metastable austenitic stainless steel and the titanium alloy Ti6Al4V. A numerical model based on the boundary-element method has been developed, where crack propagation is described by means of partially irreversible dislocation glide on crystallographic slip planes in a polycrystalline model microstructure. This concept is capable to account for the strong scatter in fatigue life for very small strain amplitudes and to contribute to the concept of tailored microstructures for improved cyclic-loading behaviour.

MM 58.3 Thu 16:30 H4

Ermüdungsrissinitiierung durch Bildung feinkörniger Bereiche bei sehr hohen Lastspielzahlen — •Eberhard Kerscher[1], Patrick Grad[1], Bernhard Reuscher[2], Alexander Brodyanski[2] und Michael Kopnarski[2] — [1]Arbeitsgruppe Werkstoffprüfung, TU Kaiserslautern, Deutschland — [2]Institut für Oberflächen- und Schichtanalytik, TU Kaiserslautern, Deutschland

Metallische Konstruktionswerkstoffe zeigen bei zyklischer Beanspruchung im Bereich sehr hoher Lastspielzahlen veränderte Schädigungsmechanismen: so tritt in höchstfesten Stählen keine ausgeprägte Wechselfestigkeit auf, sondern es ist ein Versagen durch Rissinitiierung von inneren Einschlüssen zu beobachten. Typisch für das Versagen ist dabei die Bildung eines kreisrund ausgeprägten Ermüdungsrisses direkt um den Einschluss (fish-eye). Bei sehr langen Lebensdauern findet sich zusätzlich direkt um den Einschluss ein feinkörniger Bereich. Zur Erklärungen möglicher Bildungsmechanismen wurden, zusätzlich zu Bruchflächenuntersuchungen im REM, die feinkörnigen Bereiche, die nach Ermüdungsversuchen an martensitischen und bainitischen Zuständen des Stahls 100Cr6 entstanden waren, detaillierter analysiert. Dazu wurden zuerst definierte Bereiche der Mikrostruktur um rissinitiierende Einschlüsse mittels focused ion beam (FIB) freigelegt und anschließend im REM und im TEM analysiert. Ausgehend von diesen Untersuchungen wird ein neues Modell vorgeschlagen, mit dem sich alle bisherigen Untersuchungsergebnisse hinsichtlich der Bildung des feinkörnigen Bereiches sowie der Rissentwicklung durch diesen Bereich erklären lassen.

MM 58.4 Thu 16:45 H4

R-curve characteristics of Zr-based bulk metallic glasses — •Davide Granata, Samuele Laffranchini, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

In light of the utilization of bulk metallic glasses (BMGs) as structural materials the fracture toughness has to be significantly enhanced. Thereby, it is of great importance to gain a better understanding of the experimental and structural factors governing the resistance to fracture. However, only a few BMGs with high fracture toughness values have been developed so far. Due to limited sample thickness and major difficulties concerning the controlled introduction of a straight fatigue pre-crack most of these investigations do not follow the standard ASTM test methods. Most recently, feasible R-curves of ductile Pd- and Zr-based BMGs have been measured yielding promising values comparable to conventional steel and crystalline titanium alloys respectively. In this study, results relating to the implementation of R-curves in the Zr-Cu-Al ternary and Zr-Cu-Al-Ta quaternary system are reported. To this effect, conclusions on the most important experimental parameters are presented and the measured fracture toughness values are related to bonding characteristics.

MM 59: Computational Materials Modelling - Phase Stability III

Time: Thursday 15:45–17:00 Location: H24

MM 59.1 Thu 15:45 H24

Phase diagram of Cr_xSb_y - A theoretical study on the structural and magnetic properties — •Gerhard Kuhn[1], Svitlana Polesya[1], Sergiy Mankovsky[1], Hubert Ebert[1], Matthias Regus[2], and Wolfgang Bensch[2] — [1]Ludwig-Maximilians-Universität München — [2]Christian-Albrechts-Universtität zu Kiel

We present results of first-principles investigations on the electronic structure, magnetic properties and phase stability of stoichiometric Cr_xSb_y compounds. The work is based on electronic structure calculations performed within the frame of DFT. The magnetic properties at finite temperature are studied using the Monte Carlo method based on the Heisenberg model.

The focus will be on $CrSb_2$ with marcasite structure exhibiting interesting electronic and magnetic properties. GGA as well as GGA+U calculations have been performed to show the role of local correlation effects, for electronic and magnetic properties. Comparing different types of magnetic order - i.e. ferromagnetic (FM) and antiferromagnetic (AFM) order along different directions - we have found in accordance with experiment the AFM order to be the stable one. Furthermore total energy calculations show a phase transition from marcasite to $CuAl_2$-structure for hight pressures according to experimental investigations.

Different types of structures are considered for the Cr_3Sb phase that is observed in several experiments. Total energy calculations for the most probable structures were performed to compare their stabilities and properties.

MM 59.2 Thu 16:00 H24

Rationalizing and screening high throughput DFT calculations using systematic tight binding models of transition metal - group 14 compounds. — •Alessandro Parma, Eunan J. McEniry, Ingo Opahle, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum Universität Strasse 90a, 44789 Bochum, Germany

High throughput Density Functional Theory calculations are a powerful tool in materials design, since they allow for the discovery of new stable structures with relevant electronic or mechanical properties.

We rationalize the phase stabilities of transition metal-group 14 compounds based on systematically derived orthogonal Tight Binding (OTB) models. The optimized minimal basis is obtained by downfolding a multiple-ζ LCAO basis. The bond integrals within the two center approximation are then calculated from this down-folded DFT Hamiltonian. They are found to be continuous and transferable and show trends across the transition metal period, allowing us to implement a general *pd* OTB model.

Our focus will be on the prediction of structural stabilities in terms of number of electrons in the *d* shell and principal quantum number of the *p*-states. An efficient screening strategy is developed based on the structural energy difference theorem. A reliable OTB model that reproduces DFT trends is crucial in the framework of high throughput structure search, since it allows for much more efficient energy calculations.

MM 59.3 Thu 16:15 H24

Phase diagram and thermodynamic properties of aluminum nitride from *ab initio* calculations — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The AlN system is of interest in the context of phase diagram studies of the Si–Al–O–N system where AlN is one important binary compound. Recent experiments have generated interest in the calculation of a *P-T* phase diagram for the AlN system in order to supplement the avaliable *ab initio* based data.

We used density functional perturbation theory in order to obtain the phonon density of states and the quasi-harmonic approximation to calculate thermodynamic properties of the low pressure wurtzite and high pressure rocksalt phase.

We present results on the *P-T* behavior of thermodynamic properties (heat capacity, bulk modulus, thermal expansion) and compare to experimental data. Especially, we show how the anisotropic thermal expansion of the wurtzite phase is calculated. A phase diagram constructed from calculated Gibbs enthalpy data for the wurtzite - rocksalt phase transition is presented. We also discuss the limits of the method and report results regarding the thermal stability of the high pressure phase.

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

MM 59.4 Thu 16:30 H24

Structure optimization via "local heat pulse"-quench cycles — •Arnulf Möbius[1] and Christian Schön[2] — [1]Institute for Theoretical Solid State Physics, IFW, Dresden — [2]Max Planck Institute for Solid State Research, Stuttgart

Structure prediction for crystals with a large number of atoms in the primitive cell, as well as for clusters of many atoms, are often impeded by the corresponding energy landscape exhibiting a huge number of local minima. For such tasks, we present an optimization procedure which is based on "local heat pulse"-quench cycles (LHPQC). It was originally developed for combinatorial optimization tasks [1].

This approach is applied to a lattice structure prediction problem. In that, we use the general utility lattice program (GULP) by J.D. Gale and co-workers [2] as local search code. As a test case, the energy landscape of the $Mg_{10}Al_4Ge_2Si_8O_{36}$ lattice is investigated, where the interactions are modelled by Coulomb, Buckingham, and three-body potentials [3], and where the cell parameters are free to vary.

The results of our computer experiments testify that the LHPQC procedure is robust and far more efficient than the previous approaches to the same test problem in Ref. 3. Finally, we show how our procedure can be easily parallelized: Its efficiency is considerably improved by treating an ensemble of local minima instead of a single one.

[1] A. Möbius, A. Neklioudov, et al., Phys. Rev. Lett. 79 (1997) 4297.
[2] J.D. Gale and A.L Rohl, Mol. Simul. 29 (2003) 291.
[3] A.R. Oganov, J.C. Schön, et al., in "Modern methods of Crystal Structure Prediction", ed. A.R. Organov, (Wiley, 2011), p. 223.

MM 59.5 Thu 16:45 H24

Improving the magneto-caloric effect in layered alloys: an ab-initio investigation — •Biswanath Dutta[1], Tilmann Hickel[1], Jörg Neugebauer[1], and Andreas Hütten[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany — [2]Department of Physics, Thin Films and Physics of Nanostructures, Bielefeld University, PB 100131, 33501 Bielefeld, Germany

The study of magnetocaloric effect (MCE) based magnetic refrigeration is primarily focused on increasing the magnetic entropy difference ΔSmag(H,T) between the two phases across the coupled magnetic and structural transition. Here, we demonstrate a novel strategy consisting of alternating layers of different magnetocaloric materials. For this study, we choose Heusler alloys Ni-Mn-Sn and Ni-Mn-Ga for which the details of MCE in the bulk phase are well investigated. The presence of different chemical species across the interface in the layered structure, however, opens up the possibility of significant changes in the magnetic and structural properties which we investigate with the help of density functional theory. Our calculations reveal that the atomic magnetic moments get modified near the interface leading to the conclusion that interfaces could influence the transition temperatures and the entropy change and thus alter the MCE. In order to further clarify this influence, we carefully investigated strain contributions, interlayer diffusion and possible segregation effects near the interface.

MM 60: Nanomaterials - Nanoparticles

Time: Thursday 15:45–17:00 Location: H25

MM 60.1 Thu 15:45 H25

Tuning of silver ion release properties of silver-polymer nanocomposites — •Nisreen Alissawi, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — Institute for Materials Science - Multicomponent Materials, Faculty of Engineering, Christian-Albrechts-University (CAU) Kiel, Kaiser Str. 2, 24143, Kiel, Germany

The tuning of silver ion release is very important for biomedical applications of silver nanocomposite materials to reduce the potential toxicity effects towards human cells and the environment. In this work a well defined model system consisting of nearly two dimensional silver nanoparticle ensembles deposited on the surface of a polymer matrix was used to study the influence of different parameters on the silver ion release. Samples were prepared by physical vapor deposition (PVD) techniques. The effect on Ag ion release kinetics was investigated in dependence of the composite morphology (Ag nanoparticle size, concentration, and distribution), for nanocomposites containing silver (Ag) and gold (Au) as alloy nanoparticles with different composition, or with a polymer barrier on top of the NPs. Composition and the time-dependent release of silver ions after immersion in water were examined by a combination of techniques. Increasing the gold fraction

in Ag-Au alloy NPs leads to a strong improvement of the oxidation resistance of the AgNPs. Moreover, a polymer barrier stabilizes the morphology of the composites and allows controlling the Ag ion release rate.

MM 60.2 Thu 16:00 H25

Role of oxygen on stabilization of TiOx cluster production by gas aggregation cluster source — •Amir Mohammad Ahadi[1], Vladimir Zaporojtchenko[1,3], Alexander Martin Hinz[1], Tilo Peter[1], Oleksandr Polonskyi[2], Thomas Strunkus[1], and Franz Faupel[1] — [1]Faculty of Engineering, Institute for Material Science, Multicomponent Materials, Christian Albrechts University, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]deceased on 31.08.2012

Reactive DC magnetron sputtering from a Ti target combined with a gas aggregation chamber was applied to form TiOx clusters. Continuing previous work [1] the role of oxygen (as a reactive gas) on stabilization of TiOx cluster formation has been investigated. It was observed that at appropriate sputter conditions and by adding a certain oxygen flow, high and stabilized cluster deposition can be achieved. But already small changes of the oxygen flow lead to unstable cluster deposition rates. Further experiments at different magnetron power showed that the required oxygen flow for stabilization of the cluster deposition rate depends strongly on the magnetron power used. Analysis of the escaped oxygen concentration - from aggregation chamber as determined by mass spectrometry- indicates the crucial role of the reactive gas for cluster formation on the one side and poisoning of the target on the other side.

[1] T. Peter, O. Polonskyi, B. Gojdka, A.M. Ahadi, T. Strunskus, V. Zaporojtchenko, H. Biederman, F. Faupel, J. Appl. Phys., accepted(2012).

MM 60.3 Thu 16:15 H25

Magnetic Memory Effect in Chelated Zero Valent Iron Nanoparticles — •Nilotpal Ghosh, Badal Kumar Mandal, and Kesarla Mohan Kumar — School of Advanced Sciences, VIT University, Vellore-632014, Tamilnadu, India

We report the study of non-equilibrium magnetic behaviour of air stable Zero Valent Iron Nanoparticles synthesized in presence of N-cetyl-N,N,N-trimethyl ammonium bromide chelating agent. X-ray photoelectron spectroscopy study has suggested the presence of Iron oxides on nZVI surfaces. Zero-field-cooled and field-cooled magnetization measurements have been carried out at 20-300 K and 100 Oe. For field-cooled measurements with 1hr stops at 200, 100 and 50 K when compared with the warming cycle, we found the signature of magnetic memory effect. A study of magnetic relaxation at same the temperatures shows the existence of two relaxation times.

Reference : N. Ghosh, B.K. Mandal, K. M. Kumar, Journal of Magnetism and Magnetic materials 324 (2012)3839.

MM 60.4 Thu 16:30 H25

Synthesis and characterization of magnetic core-shell nanoparticles — •Marcel Hennes[1], Andriy Lotnyk[1], and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM), Leipzig, Germany — [2]Translationszentrum für Regenerative Medizin (TRM), Universität Leipzig, Germany — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Magnetic nanoparticles with an inert functionalizable shell have received increasing attention during the past years, owing to their application potential e.g. in medicine or catalysis. In the present contribution, we report about our approaches to synthesize tailored magnetic core-shell nanoparticles using plasma assisted inert gas condensation (PA-IGC). Employing Cu/Ni as example of a binary alloy with moderate miscibility gap and different surface energies of the constituents, we first address the potential of synthesizing rotationally symmetric core-shell structures by self-organization using a combined Monte-Carlo / Molecular Dynamics computer simulation approach based on different well-established embedded atom method (EAM) potentials. Our results indicate presence of a Cu segregation layer of about one monolayer thickness, but absence of spherically symmetric core-shell particles. Motivated by these findings, an experimental setup with a post-synthesis coating stage is presented, that is capable of producing fine-tuned core-shell magnetic structures, as verified with aberration corrected high resolution transmission electron microscopy.

MM 60.5 Thu 16:45 H25

Size-dependent evolution of the phonon density of states of isolated Fe nanoparticles — Beatriz Roldan Cuenya[1], Luis K. Ono[1], Jason R. Croy[1], Kristof Paredis[1], Abdelkader Kara[1], Jiyong Zhao[2], Ercan E. Alp[2], and •Werner Keune[3,4] — [1]Department of Physics, University of Central Florida, Orlando, FL, USA — [2]Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA — [3]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [4]Max-Planck Institute of Microstructure Physics, Halle, Germany

The phonon density of states [PDOS, g(E)] of self-assembled isolated 57Fe nanoparticles (NPs) (2-6 nm in size) on SiO2/Si(111) substrates, synthesized by inverse micelle encapsulation, was measured as a function of NP size by nuclear resonant inelastic X-ray scattering (NRIXS) of synchrotron radiation. The NPs were protected by a Ti coating layer. An intriguing behavior was observed: an increase of the low-energy excess PDOS (as compared to bulk bcc Fe) with increasing NP size, combined with Debye behavior [g(E) prop. E^n, with n = 2] for small NPs (2 nm), but non-Debye behavior (n = 1.4) for larger NPs. This unexpected result can be qualitatively explained by the existence of low-coordinated Fe atoms located at grain boundaries and other defects with structural disorder in the interior of the large NPs, but not in the small NPs (2 nm). The PDOS was used to calculate important thermodynamic quantities of Fe nanoparticles, such as the atomic mean-square vibrational displacement, vibrational specific heat and vibrational entropy.

MM 61: Liquid & Amorphous Metals I

Time: Thursday 15:45–17:00 Location: H26

MM 61.1 Thu 15:45 H26

Density and viscosity of Cr-Fe-Ni ternary liquid alloys — •Hidekazu Kobatake and Juergen Brillo — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

Materials of practical relevance, such as Fe-based alloys or stainless steels are mainly ternary combinations of Cr, Fe and Ni. Density and viscosity of these liquid metals are required to simulate the buoyancy forced convection in a liquid during the welding and casting process. Especially, density is required as input parameter for the calculation of other thermophysical properties from the primary measurement data. In this study, the density was measured using electromagnetic levitation as a container-less technique. The shadowgraph of the sample was captured by digital CCD camera and its volume was calculated to by an image processing algorithm to determine the density. In the measured concentration range, the excess volume is positive. The experimentally obtained densities of the ternary system agree well with those calculated according to a thermodynamic mixing rule taking into account contributions from the binary margin systems only. Viscosities, η have been measured by means of a high-temperature oscillating cup viscometer. A cylindrical cup which contains the liquid sample is suspended by a torsion wire and is oscillated around its vertical axis. η was then obtained from the decrement of the oscillation. In the investigated compositional range of the Cr-Ni-Fe system, η as a function of temperature can be described by an Arrhenius law. Isothermal viscosities will be compared to existing thermodynamic models.

MM 61.2 Thu 16:00 H26

Phase separation in liquid and amorphous metallic alloys — •Norbert Mattern[1], Junhee Han[1], Ulla Vainio[2], Ahmed Shariq[3], Pradeep Konda Gokuldoss[4], Dierk Raabe[4], and Jürgen Eckert[1,5] — [1]IFW Dresden, Institute for Complex Materials — [2]Hasylab at Desy, Hamburg — [3]FhG Center Nanoelectronic Technology, Dresden — [4]MPI für Eisenforschung,Düsseldorf — [5]TU Dresden,Institute of Materials Science

Phase-separated glasses are well known for oxide glasses and polymers. In the last years two-phase glasses were successfully prepared in different metallic alloy systems by rapid quenching from the melt. We

report recent results on the influence of composition and casting conditions on the phase separation and the structure formation of glass forming metallic alloys Zr-M-Al-Gd (M =Cu,Co,). The decomposition in such alloys is a consequence of the large positive enthalpy of mixing between Zr and Gd (Hmix= +9 kJ/mole). We will show that early stages of spinodal decomposition can be obtained if the critical temperature of liquid-liquid phase separation is near to the glass transition temperature. Evidence of formation of Gd-enriched clusters by a spinodal mechanism is obtained by small-angle X-ray scattering and atom probe tomography.

MM 61.3 Thu 16:15 H26

Phase separation in ternary Co-Gd-Ti liquids — •Junhee Han[1], Norbert Mattern[1], Dirk Holland-Moritz[2], Jozef Bednarcik[3], Ivan Kaban[1], Rafal Nowak[4], Natalia Sobczak[4], and Jürgen Eckert[1] — [1]IFW-Dresden, Dresden, Germany — [2]Institut für Materialphysik im Weltraum, DLR, Köln, Germany — [3]HASYLAB, DESY, Hamburg, Germany — [4]Center for High Temperature Studies, Foundry Research Institute, Krakow, Poland

Phase equilibrium and solidification behavior of ternary Co-Gd-Ti (Co $\leq$ 35 at. %) alloys has been investigated by thermal analysis (DSC) and microstructural characterization of cast alloys (SEM/EDX). The phase equilibria with the liquid phase were studied in situ for two alloys $Co_{30}Gd_{35}Ti_{35}$ and $Co_{30}Gd_{50}Ti_{20}$ by combining electrostatic levitation of the melt with high-energy synchrotron X-ray diffraction at elevated temperature. For $Co_{30}Gd_{35}Ti_{35}$ we observe two diffuse diffraction maxima (T = 1600 - 1700 K) giving direct evidence of liquid-liquid phase separation. The maxima positions exhibit a temperature dependent shift due to the change in chemical compositions with temperature in accordance with the binodal line. For $Co_{30}Gd_{50}Ti_{20}$, no indication of phase separation is detected. Coarsened microstructures typically for phase separated liquids are observed in cast alloys $Co_{30}Gd_{35}Ti_{35}$, $Co_{25}Gd_{37.5}Ti_{37.5}$, $Co_{10}Gd_{45}Ti_{45}$ and $Co_{30}Gd_{20}Ti_{50}$. Our findings suggest that the stable miscibility gap of the binary Gd-Ti extends into the ternary Gd-Ti-Co system (up to Co < 35 at. %). Thermodynamic calculations of the ternary Co-Gd-Ti by the CALPHAD method are in a good agreement with experimental findings.

MM 61.4 Thu 16:30 H26

Crystallisation and glass transition of a AuSi based metallic glass investigated by chip based ultra fast scanning calorimetry — •Joachim Bokeloh, Jonas Bünz, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

The glass transition as well as the crystallization of metallic glasses have been extensively studied in the past. These investigations are limited by two experimental issues. For one, the complex relationship between intrinsic properties of the material and its time-temperature history renders the state of cast samples somewhat ambiguous. Secondly, conventional laboratory equipment is incapable of exploring the broad dynamic range that is of interest in the case of metallic glasses.

We present here measurements of a AuSi based metallic glass by chip-based ultra fast scanning calorimetry (50K/s - 10 000 Ks). The high heating and cooling rates allow for a highly controlled and repeatable in-situ vitrification of a glassy sample, investigation of the glass transition during heating as well as cooling at various rates and an in-depth analysis of the crystallization behaviour when cooled down from the melt, as compared to when heated up from the glassy state.

MM 61.5 Thu 16:45 H26

Reactive wetting and solder spreading — •André Wedi and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

Wetting is an important pre-requisite of a reliable solder connection. However, it is only an indirect measure for the important specific energy of the reactive interface between solder and base metallization of Cu and Ni. In order to quantify this energy, we measured wetting angles of solder drops as well as surface tension of SnPb and SnBi solders under systematic variation of composition and gaseous flux at different reflow temperatures by the sessile drop method. Remarkably, the tension between solder and flux and the wetting angle reveal characteristic dependence on solder composition. From the two independent data sets, the specific energy of the reactive interface, the adhesion tension, is evaluated. In detail, the adhesion energy reveals distinguished plateaus which are related to different reaction products in contact to the solder. Using a dedicated geometry [1], which enables investigation of the wetting kinetics, spreading speed and maximum spreading distance are measured. We demonstrate correlations between the latter kinetic parameters and the phase structure in the reaction zone.

[1] F.M. Hosking et al, Journal of Electronic Materials, Vol. 25, No. 7, 1996.

MM 62: Topical Session: Fundamentals of Fracture - Stochastic Aspects

Time: Thursday 17:15–18:45 Location: H4

Topical Talk MM 62.1 Thu 17:15 H4

Elasticity and disorder for fracture size effects — •Stefano Zapperi — IENI-CNR, Milano, Italy — ISI foundation, Torino,Italy

I will discuss the asymptotic properties of fracture strength distributions of disordered elastic media studied by combination of renormalization group, extreme value theory, and numerical simulation. We investigate the validity of the weakest-link hypothesis in the presence of realistic long-ranged interactions in the random fuse model. Numerical simulations indicate that the fracture strength is well-described by the Duxbury-Leath-Beale (DLB) distribution which is shown to flow asymptotically to the Gumbel distribution. We explore the relation between the extreme value distributions and the DLB-type asymptotic distributions and show that the universal extreme value forms may not be appropriate to describe the nonuniversal low-strength tail. Finally, we confirm numerically that the Weibull distribution, widely used in the past to fit failure statistics from experiments, only arises when the distribution of pre-existing disorder has a power law tail and is otherwise unstable due to interactions.

MM 62.2 Thu 17:45 H4

Time evolution of creep rupture due to thermally activated cracking in a fiber bundle model — •Ferenc Kun[1], Naoki Yoshioka[2], and Nobuyasu Ito[3] — [1]Department of Theoretical Physics, University of Debrecen, P.O.Box: 5, H-4010 Debrecen, Hungary — [2]Yukawa Institute for Theoretical Physics, Kyoto University, Kitashirakawa Oiwake-cho, 606-8502 Kyoto, Japan — [3]Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan

We study sub-critical fracture driven by thermally activated crack nucleation under a constant external load in the framework of fiber bundle models. We show that in the presence of stress inhomogeneities, thermally activated cracking results in an anomalous size effect, i.e. the average lifetime of the system decreases as a power law of the system size, where the exponent depends on the external load and on the temperature.

On the microlevel, thermal fluctuations trigger bursts of breakings which proved to have a power law size distribution. Focusing on the waiting times between consecutive bursts we show that the time evolution has two distinct forms: at high load values the breaking process continuously accelerates towards macroscopic failure, however, for low loads and high enough temperatures the acceleration is preceded by a slow-down. Analyzing the structural entropy and the location of consecutive bursts we show that in the presence of stress concentration the early acceleration is the consequence of damage localization.

MM 62.3 Thu 18:00 H4

Failure Prediction in Silicon Nitride based on a Probabilistic Micromechanical Approach — •Yamen Othmani and Thomas Böhlke — Chair for Continuum Mechanics, Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Kaiserstrasse 10, 76131 Karlsruhe, Germany

Silicon nitride ceramics are prime structural materials for several challenging assignments and applications. This is due to their outstanding high stiffness, high-temperature strength and, especially, their high fracture toughness. However the structural use of these materials is restrained because of the occurrence of damage phenomenon under severe working conditions. Many approaches, including fracture mechanics, could be adopted to predict the failure of silicon nitride. Nev-

ertheless, the strengths of such materials are statistical in nature and the damage progression is stochastic. Therefore, the application of statistical methods to evaluate the failure of ceramics is a versatile approach. In the present work, multivariate weakest link approach is developed and used in conjunction with a stochastic analysis of the local elastic fields to determine the failure probability of sintered silicon nitride. The originality of the work is reflected by the employment of second-order estimates in the analysis of elastic field fluctuations. The following assumptions have been taken into consideration: The constitutive phases of silicon nitride are considered to be isotropic and linear elastic. The strain field is compatible which implies a vanishing distribution of eigenstresses.

MM 62.4 Thu 18:15 H4

Thermally Activated Fluctuating Dynamics of Dislocations in a Low-Stress Zone — •Thomas Swinburne — EURATOM/CCFE Fusion Association, OX14 3DB — Department of Physics, Imperial College London, SW7 2AZ

A crack is an intense dislocation source, and the propagation of the crack is controlled by the mobile dislocations forming the atmosphere extending into the far-field low stress zone. The mobility of dislocations is believed to control brittle to ductile transition [Hirsch, Roberts and Samuels 1989, Hartmaier and Gumbsch 1999].

To explore the transition from brittle to ductile fracture it thus becomes essential to investigate dislocation mobility under vanishing applied stress, a regime typically considered inaccessible to atomistic simulation of bcc metals due to the kink limited motion of screw dislocations. This is overcome through specially adapted large-scale atomistic simulations which enforce the existence of individual kinks on a dislocation line. The temperature dependence of the resultant kink motion contradicts decades of theoretical work and leads to new conclusions on dislocation friction.

A stochastic line model is capable of quantitatively capturing the diverse range of temperature dependent effects seen in atomistic simulation providing the line is crystallographically discrete, introducing a new length scale into thermally activated plasticity. The model, fully parametrised from atomistic simulation, is used to predict the thermally activated response of mobile dislocations to vanishing applied stress.

MM 62.5 Thu 18:30 H4

The low temperature deformation properties of thermally active bulk metallic glasses — •Peter Derlet — Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland

Despite significant atomic-scale heterogeneity, bulk metallic glasses well below their glass transition temperature exhibit a sharp transition to plasticity with a reproducible yield stress. Under tension, limited ductility is observed with the materials often exhibiting brittle fracture. Because of the high reproducibility of the yield stress such mechanical failure is not flaw based (as in a ceramic) but rather an intrinsic property of the structural glass. The present work investigates these issues via a thermal activation model which assumes the number of available irreversible structural transformations scales exponentially with an internal heterogeneous length scale. It is found that a distinct low temperature deformation regime exists which is dominated by the statistics of kinetic freezing, giving an approximately linear increase in yield stress as a function of decreasing temperature. This result is discussed in terms of the onset of heterogenous plasticity and eventual macroscopic material failure.

MM 63: Computational Materials Modelling - Phase Stability IV

Time: Thursday 17:15–19:00 Location: H24

MM 63.1 Thu 17:15 H24

A thermodynamic consistent multi-phase-field model base on the maximal entropy production principle — •haifeng wang and herlach d.m. — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

The maximal entropy production principle (MEPP) based on which the additional constrains can be incorporated conveniently by the Lagrange method is applied to propose a new multi-phase-field model. The phase-field and diffusion equations follow the classical Onsanger reciprocal law which means that the present work is thermodynamic consistent with the classical irreversible thermodynamics. The bulk and interface contributions can be separated completely both at equilibrium condition and highly non-equilibrium condition where complete solute trapping happens. For medium growth velocities, the interaction between the bulk and interface contributions can be suppressed by increasing the order of a new interpolation function, which makes a quantitative modeling of rapid solidifications possible. For the one-sided growth model, the driving force for the phase field is not the grand potential but the model with solute drag as is in the classical sharp interface model. This means that the grand potential function which does not incorporate the additional constrains rightly is not thermodynamics consistent. Application to rapid solidification Si-9at.%As alloy shows that a good agreement between the model prediction and experimental results can be found.

MM 63.2 Thu 17:30 H24

Real-time observation of Ostwald ripening by synchrotron tomography — •Thomas Werz[1], Michael Heinze[2], Lukas Helfen[3], Mario Scheel[4], Stefan Odenbach[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Institute of Fluid Mechanics, TU Dresden, Germany — [3]ESRF ID19, Grenoble, France — [4]ESRF ID15A, Grenoble, France

Synchrotron tomography is an ideal tool for the time-resolved, three-dimensional observation of coarsening phenomena like Ostwald ripening. In contrast to classical grain growth, in which grain boundaries migrate in a single-phase material, Ostwald ripening entails particle growth and shrinkage in the presence of at least two phases, and the evolution of the microstructure depends sensitively on the volume fraction of the coarsening phase, V_V. In the present study we focus on capturing the coarsening behavior at such high values of V_V that the system might manifest signs of a transition between Ostwald ripening and grain growth ($V_V = 1$). For this purpose, we designed a sample furnace that is compatible with the optical constraints of x-ray tomography, enabling precise control over V_V in a two-phase AlCu alloy by adjusting the temperature. After applying various image processing and segmentation steps to the reconstructed tomographic data, we extract both local and global features of the microstructure and follow their evolution with time.

MM 63.3 Thu 17:45 H24

Relaxor behavior of ferroelectric Ca0.22Sr0.12Ba0.66Nb2O6 single crystals — •Chandra Shekhar Pandey[1], Jürgen Schreuer[1], Manfred Burianek[2], and Manfred Mühlberg[2] — [1]Institute of Geology, Mineralogy and Geophysics, Ruhr-Universität Bochum, Universitaetsstrasse 150, 44801-Bochum, Germany — [2]Institute of Crystallography, Greinstrasse 6, 50939-Cologne, Germany

The relaxor behavior of tetragonal tungsten bronze uniaxial relaxor ferroelectric calcium strontium barium niobate (Ca0.22Sr0.12Ba0.66Nb2O6 or CSBN22) single crystal was studied by measuring elastic constants and thermal expansion with the aid of resonant ultrasound spectroscopy and dilatometry respectively, in the temperature range 300 K upto 1503 K. Thermal expansion yields evidence of the Burns temperature TB, and the intermediate characteristic temperature T*, which was also supported by the temperature evolutions of the elastic constants cij. CSBN22 was found to be about 2-3 % elastically stiffer than CBN28. The presented results open the perspective to understand the relaxor behavior in CSBN.

MM 63.4 Thu 18:00 H24

Acoustic emission during the martensitic transformation of a Ni-Mn-Ga single crystal under compressive stress — •Robert Niemann[1,2], Jordi Baró[3], Oleg Heczko[4], Ludwig Schultz[1,2], Sebastian Fähler[1,2], Eduard Vives[3], Lluis Mañosa[3], and Antoni Planes[3] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Department of Physics, Institute for Solid State Physics, Dresden University of Technology, 01062 Dresden, Germany — [3]Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona. Diagonal 647, 08028 Barcelona,

Catalonia, Spain — [4]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic

The propagation of a phase front during a thermally induced martensitic transition is discontinuous due to pinning at various defects, an effect which results in acoustic emission. Here we analyze the consequences of an applied compressive stress exemplarily on a Ni-Mn-Ga single crystal. Our experiments show that the distribution of the energies of the acoustic emission events follows a power law for more than 3 decades. This indicates that the transition exhibits avalanche criticality. The exponent characterizing the distribution of energies depends on the applied stress and decreases from 1.9 at zero stress to 1.5 at stress above 3 MPa. This decrease could be attributed to the reduced multiplicity of variants possible under uniaxial compression.

MM 63.5 Thu 18:15 H24

Inverse magnetocaloric effect of epitaxial Ni-Mn-based films — •Anett Diestel[1], Robert Niemann[1,2], Maximilian Uhlmann[1,2], Ludwig Schultz[1,2], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute of Materials Science, 01062 Dresden, Germany

The Heusler alloys Ni-Mn-X (X = Ga, In, Sn, Sb) have been identified as versatile functional materials. Due to the diffusionless phase transformation from austenite to martensite, which can be induced by magnetic field, the materials show the (inverse) magnetocaloric effect (MCE). They are promising materials for magnetocaloric cooling devices at room temperature application. Due to the high surface-to-volume ratio of thin films a fast heat exchange and a higher cycle frequency is possible. Therefore higher cooling efficiency can be achieved using less material compared to bulk. We prepared epitaxial Ni-Co-Mn-In [1] and Ni-Mn-Ga-Co films by magnetron sputter deposition on single crystalline MgO(100). For both materials we proved epitaxial growth and the reversible transformation from ferromagnetic austenite to modulated, non-ferromagnetic martensite. For Ni-Co-Mn-In an inverse MCE with an entropy change of 8.8 J/(kgK) at 9 T near room temperature was achieved.[1] By adding Co the martensitic transformation and the Curie temperatures can be shifted to maximize the inverse MCE at room temperature. The results show that epitaxial Ni-Mn-based films are promising materials for efficient magnetocaloric cooling devices. [1] R. Niemann et al. Appl. Phys. Lett. 97, 2010

MM 63.6 Thu 18:30 H24

Ion-Irradiation-Assisted Phase Selection in Single Crystalline Fe7Pd3 Ferromagnetic Shape Memory Alloy Thin Films: From fcc to bcc along the Nishiyama-Wassermann Path — •Ariyan Arabi-Hashemi[1] and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V., Leipzig, Germany — [2]Translationszentrum für Regenerative Medizin, Universität Leipzig, Germany — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Fe7Pd3 exhibits four different metastable phases: the austenite fcc phase and three martensite phases (fct, bct, and bcc). Our work aims at exploring the influence of generalized internal stresses due to (i) point defects and (ii) deviations from equilibrium short-range order. While the former are stresses in a strict mechanical sense, the latter are the conjugate variable of the short-range order parameter. In a given sample, manipulation of both, (i) and (ii) can conveniently be achieved by means of irradiation with energetic ions. 500 nm thick single crystalline Fe7Pd3 films were deposited at 850°C on MgO (001) single crystalline substrates. The unirradiated samples exhibit prevalently the austenite fcc phase. These thin films were ion-irradiated with 1.8 MeV Kr+ -ions. Fluency dependant T2T-measurements show that ion-irradiation-assisted phase selection along the whole transformation path ranging from fcc->bcc is possible. Fluency dependant pole figure measurements describe the fcc->fct and the transformation into the bcc phase in detail. An orientation relationship according to Nishiyama-Wassermann for the fcc->bcc transformation is observed.

MM 63.7 Thu 18:45 H24

Study of RGS (Ribbon Growth on Substrate) microstructure development — •Pierre Yves Pichon[1,2], Dieter Herlach[1], Schönecker Axel[2], Dirk Holland-Moritz[1], and Matthias Kolbe[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe 51170 Köln — [2]RGS Development B.V. Bijlestaal 54 A 1721 PW Broek op Langedijk The Netherlands

Silicon wafer for solar cell applications can be produced at high speed and in one step by the RGS technique. Textured substrates at initial temperature below the melting point of silicon are moved at a constant speed under a silicon bath, providing the driving force for nucleation and crystal growth. Heat extraction is perpendicular to the wafer transport; therefore production rate is decoupled from crystallization velocity. The development of the microstructure is strongly influenced by the thermal-mechanical contact interface between the wafer and the substrate: the summits of the substrate surface texture make discrete contact points with the wafer. It was found that a better contact leads to higher growth velocity, smaller grain size and higher dislocation density. The important parameters influencing the formation of the interface were studied during casting experiments and by bringing silicon droplets in contact with the substrate. It was found that the initial temperature of the substrate is strongly influencing the formation of the thermal contact. Under certain conditions it was found that the crystallization front can form twinned dendritic crystals. This was attributed to a higher driving force for crystal growth than the driving force for nucleation on the substrate.

MM 64: Nanomaterials - Miscellaneous

Time: Thursday 17:15–18:45 Location: H25

MM 64.1 Thu 17:15 H25

Plasmon resonances in Janus particles — •Sol Carretero-Palacios, Frank Jäckel, Theobald Lohmüller, and Jochen Feldmann — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Department of Physics and Center for Nano-Science (CeNS), Amalienstr. 54, D-80799, München, Germany

Janus particles are particles whose surfaces have two or more different types of properties. Standard Janus particles used for optical manipulation consist of micro-silica core spheres half-coated with gold. The spherical asymmetry associated with Janus particles is the key point in many applications, including electrophoretic displays, nanoviscometers, and self-propelling micromachines. These systems possess a tunable plasmon resonance that can be controlled by changing the ratio of the core radius to the coating thickness.

We evaluate theoretically the extinction spectra of silica-gold Janus particles diluted in water, using a three-dimensional finite difference time domain (FDTD) method. We are able to tune the plasmon resonance from the near infrared to the optical regime by: i) half-coating the silica sphere with gold, but reducing the radius of the dielectric particle; ii) half-coating the silica particle with gold, but varying the ratio between radius and coating thickness; and iii) keeping both the radius and thickness fixed, but creating Dot-Janus particles, i.e., Janus particles which have a metallic coating covering $< 50\%$ of their surface area.

MM 64.2 Thu 17:30 H25

xcitons in solids captured with bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory — •Sangeeta Sharma, John Kay Dewhurst, Antonio Sanna, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

he ab-initio calculation of optical absorption spectra of nano-structures and solids is a formidable task. The current state-of-the-art is based on many-body perturbation theory: one solves the Bethe-Salpeter equation (BSE). Unfortunately, solving the BSE involves diagonalizing a large matrix making this method computationally very expensive.

Time-dependent density functional theory (TDDFT) is another method able to determine neutral excitations of a system. Although formally exact, the predictions of TDDFT are only as good as the approximation of the exchange-correlation (xc) kernel. There are only a few xc-kernels which correctly reproduce the excitonic effect, but these kernels suffer from either being computationally as expensive as solving BSE or depend upon external parameters.

In our latest work we propose a new approximation[1] for xc-kernel, and demonstrate that this kernel is nearly as accurate as BSE and has the correct 1/q^2 behavior. The computation cost for the bootstrap kernel is minimal and no system-dependent external parameter is required.

1. S. Sharma, J. K. Dewhurst, A. Sanna, E. K. U. Gross, Phys. Rev. Lett., 107, 186401 (2011).

MM 64.3 Thu 17:45 H25

Electrically Tunable Optical Gap Antenna — •Kai Chen and Bert Hecht — Nano-Optics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Optical gap antennas consist of two gold nanorods separated by gaps with a few nanometers in width. It is critical and desirable for a variety of applications to be able to actively tune the plasmon resonances of the gap antennas. Here, we demonstrated electrically tunable optical gap antennas fabricated from single crystalline gold flakes by focused ion beam (FIB). The antennas are suspended in air and hence charge accumulation induced by an applied DC voltage on the antenna results in a repulsive Coulomb force between the two nanorods leading to increased gap size. This technique provides an effective means for the fabrication of active plasmonic elements and allows to implement devices in which (nano-)optical and mechanical degrees of freedom are coupled.

MM 64.4 Thu 18:00 H25

Morphology of Fiber-Coatings by Thiol-Ene Photochemisty and their Mechanical Properties at the Interface — •Christian Kuttner[1], Michaela Eder[2], Helmut Schlaad[3], Ingo Burgert[4], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany — [2]Max-Planck Institute of Colloids and Interfaces, Department of Biomaterials, 14424 Potsdam, Germany — [3]Max-Planck Institute of Colloids and Interfaces, Colloid Chemistry, 14424 Potsdam, Germany — [4]ETH Zürich, Institute for Building Materials & Empa, Wood Lab, 8093 Zürich, Switzerland

Control of the interfacial properties is crucial for inorganic-organic composites. We studied the interfacial adhesion between inorganic surfaces grafted with macromolecular coatings and a given epoxy matrix. The aim was to develop a better understanding of adhesion principles in (fiber-reinforced) composites and thus optimizing composites.

Thiol-ene photochemistry was utilized to introduce a polymeric gradient on silica-like surfaces following a two-step approach by Schlaad et al. without additional initiator. Two grafting-techniques were applied: "Grafting-from" polymerization resulted in brush-like homopolymer films, whereas, "grafting-onto" deposition was suitable for diblock copolymer attachment. Both techniques were adapted to modify fiberglass. The resulting coating morphologies were nanostructurally characterized (AFM, SEM, SE, TGA). The interfacial shear strength of modified fibers in an epoxy matrix was measured by a single fiber pull-out experiment to benchmark the non-covalent fiber-matrix construction.

MM 64.5 Thu 18:15 H25

Nanomechanical characterization of soft matter fibers — •Daniel Kluge[1], Julia Singer[2], Hans-Werner Schmidt[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, Germany — [2]Macromolecular Chemistry I, University of Bayreuth, Germany

Micro- and nanofibers are important structural elements in many functional materials. Their characterization requires highly advanced techniques beyond standard methods for macroscopic materials. In our contribution, we focus on nanoscale bending of free-standing fibers, which is suitable for a wide variety of fiber systems. We discuss major advantages of bending perpendicular and parallel to the substrate plane, especially the detailed investigation of the mechanical properties within and beyond linear elastic deformations. For the interpretation of the data, we use analytical as well as finite element models. In particular, we investigate supramolecular 1,3,5-Benzenetrisamides (BTAs), which allow combining the advantages of bottom-up and top-down techniques since they form well-defined fibers by self-assembly and melt electrospinning. We show that the morphology of self-assembled BTA fibers can be tailored via the substituents, establish mechanical structure-property relations and distinguish between size and material contributions. Furthermore, we compare self-assembled and electrospun fibers from the same BTAs and demonstrate that regardless of the preparation pathway, the fibers possess a remarkable mechanical stiffness. This is a striking result, since only supramolecular interactions and no covalent bonds are present in these systems.

MM 64.6 Thu 18:30 H25

Nanoscale materials and electronic transport: from ballistic to hopping approaches — •Velimir Meded[1,2], Angela Poschlad[2], Franz Symalla[1], Denis Danilov[1], and Igor Beljakov[1] — [1]Institute of Nanotechnology, KIT, Karlsruhe — [2]Stainbuch Centre for Computing, KIT, Karlsruhe

In recent years we have developed simulation methods that describe the conformation and electronic properties of materials built based on well-defined nanoscale constituents. The methods were used to describe ballistic in nanoscale devices. Here we discuss applications on single-molecule electronics, specifically molecular wires (metallic and organic) and the development of an atomic transistor [1,2,3,4].

Secondly, we present multiscale methods to describe function of organic light emitting diodes [5] by deploying morphology simulations with Monte Carlo methods, quantum mechanical analysis of the generated morphology, and hopping charge transport.

Finally, I will discuss the integration of these methods into a European framework for multiscale materials modelling, MMM@HPC, which aims at making general simulation methods accessible to a wide audience of interested scientists, by seamlessly integrating HPC resources from within its graphical user interface [6].

1. R, Maul, W. Wenzel, Phys, Rev. B, 80, 045424 (2009). 2. F. Xie, et al., Adv, Mat,, 22, 2033 (2010). 3. V. Meded, et al., SMALL,5, 2218 (2009). 4. V. Meded, et al., Phys. Rev. B, 83, 245415 (2011). 5. J. J. Kwiatkowski, et al., Phys, Chem. Chem. Phys., 10(14), 1852 (2008). 6. The MMM@HPC webpage: www.multiscale-modelling.eu

MM 65: Liquid & Amorphous Metals II

Time: Thursday 17:15–19:00 Location: H26

MM 65.1 Thu 17:15 H26

Study of crystallization behavior during ultrafast heating of metallic glasses — •Stefan Küchemann[1], Jonas Rübsam[1], Carsten Mahn[1], Goodwin Gibbins[4], Norbert Mattern[3], Marios Demetriou[2], William Johnson[2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Keck Laboratories of Engineering, California Institute of Technology, Pasadena, CA 91125, USA — [3]Leibniz Institut für Festkörper- und Werkstoffprüfung Dresden, 01171 Dresden, Germany — [4]University of Cambridge, Cambridge, UK

In this contribution, metallic glasses have been heated up homogeneously using a rapid capacitor discharge technique [1]. The heating rates of this technique are typically in the order of 10^6 K/s which allow experimental studies prior to the crystallization for temperatures up to the melting temperature or even suppress the crystallization completely.

In order to study the crystallization behavior of varios Zr-based glass formers, hard X-ray diffraction experiments have been performed at P07 beamline at DESY. To resolve short-time structural changes, the temporal resolution of the 2D Detector could be successfully increased up to 5 ms response time by using a newly developed chopper system.

For the metallic glass $Zr_{65}Cu_{27.5}Al_{7.5}$, the results show interesting features in the liquid state prior to the final crystalline stable phase.

Financial support by DFG within SFB 602 is gratefully acknowledged.

[1] William L. Johnson et al., Science 332, 828 (2011)

MM 65.2 Thu 17:30 H26

Decoupling of component diffusivities in glass-forming Zr-Ni-Ti-Cu-Be alloys above the melting temperature — •Sri Wahyuni Basuki[1], Fan Yang[2], Andreas Meyer[2], Klaus Rätzke[1], and Franz Faupel[1] — [1]Faculty of Engineering, Kiel, Ger-

many — [2]Inst. of Materials Physics in Space, Köln, Germany

Previous work[1] on glass forming Pd-Cu-Ni-P alloys, showed that while a vast decoupling occurs between the diffusivity of Pd and of the smaller components, 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. In order to check for the general validity of these results, we extended our investigations to the Zr-Cu-Ni-Ti-Be system. In this work, Co-57 and Zr-95 tracer diffusivities were determined in glass-forming $Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$ above the melting temperature. In particular, measurements were carried out simultaneously to minimize artefacts from diffusion barriers and to reduce absolute errors. Even at 20 K above the liquidus temperature, the diffusivities of Zr and Co differ clearly by a factor of four, while Co tracer diffusivities agree very well with diffusivities determined by quasielastic neutron scattering. This together with measurements of the time dependence of the penetration profiles demonstrates the general reliability of the measurements. The results are discussed in connection with viscosity data and the Stokes-Einstein equation in terms of imperfect equilibration of the melt.

[1] A. Bartsch et al., Phys. Rev. Lett. 104, 195901 (2010).

MM 65.3 Thu 17:45 H26

Diffusion and relaxation in a HPT-deformed Zr-based bulk metallic glass — •Jonas Bünz[1], Koichi Tsuchiya[2], Sergiy Divinsky[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, WWU Münster — [2]National Institute for Materials Science, University of Tsukuba

Metallic glasses are still an attractive object of investigation in the field of materials physics due to their outstanding mechanical properties. Hardness and yield strength exceed the values of their crystalline counterpart by far, but the applicability of metallic glasses is limited by the lack of considerable plasticity. Stress localization and the associated shear softening strongly weaken the structure, thus leading to the formation of shear bands. The structure of shear bands is still far from being understood. Due to their extreme sensitiveness to the free volume localization, the diffusion measurements by the radiotracer technique can bring further insight into the structural modifications of shear bands with respect to the amorphous matrix as well as to the conditions of slip during plastic straining. Here, we present the results of diffusion as well as relaxation experiments in HPT-deformed Zr-based bulk metallic glass.

MM 65.4 Thu 18:00 H26

Ultrastable Metallic Glass — •Hai-Bin Yu, Yuansu Luo, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Germany

Recently, some novel organic glassy materials, termed *ultrastable glasses* that exhibit remarkable thermodynamic and kinetic stabilities have been prepared by deposition techniques. These ultrastable glasses are at the low energy state on the potential energy landscape, unreachable by quenched glasses that aged for long-time. These materials are of special interest for understanding many fundamental issues regarding the nature of glasses. In this work, we prepared a series of free-standing Zr65Cu27.5Al7.5 metallic glass foils by magnetron sputtering with a very low deposition rate at different substrate temperatures. The resultant materials are homogenously amorphous and have a remarkable higher glass transition temperature Tg than a quenched glass made of the same composition. They are a kind of ultrastable metallic glass. An interesting finding is the ultrastable metallic glass can be prepared only within a narrow substrate-temperature range, from 0.7 to 0.8 Tg of the quenched glass. Above this temperature range the Tg of the deposited glass even decreases. This suggests a signature of surface enhanced relaxation dynamics, a topic currently actively discussed in glassy physics. Structural analysis shows the ultrastable metallic glasses have unique fractural-like nanostructures. H.B. Yu thanks the Alexander von Humboldt Foundation. We acknowledge support from the DFG via the SFB 602 and the Leibniz Program.

MM 65.5 Thu 18:15 H26

Atomic structure and glass-forming ability of Ni64Zr36 and Cu65Zr35 alloys — •Ivan Kaban[1,2], Pal Jovari[3], Valentin Kokotin[4], Olga Shuleshova[2], Brigitte Beuneu[5], Karel Saksl[6], Norbert Mattern[2], Jürgen Eckert[1,2], and Lindsay Greer[7] — [1]TU Dresden, Institute of Materials Science, Germany — [2]IFW Dresden, Institute for Complex Materials, Germany — [3]Institute for Solid State Physics and Optics, Budapest, Hungary — [4]Access e.V., Aachen, Germany — [5]Laboratoire Leon Brillouin, CEA-Saclay, France — [6]Institute of Materials Research, Kosice, Slovak Republic — [7]Department of Materials Science and Metallurgy, University of Cambridge, UK

Atomic structure of Ni64Zr36 and Cu65Zr35 alloys in glassy and crystalline states has been investigated by different experimental techniques (X-ray diffraction, neutron diffraction with isotopic substitution, extended X-ray absorption spectroscopy) and theoretical methods (reverse Monte-Carlo simulation, molecular dynamics modelling, Voronoi analysis) to explain the differences in the glass-forming abilities of these two compositions. It is established that the Ni64Zr36 glass is characterized by pronounced topological and chemical ordering, while the Cu65Zr35 glass is topologically ordered and chemically rather disordered. Remarkably large differences in the partial pair distribution functions for the Cu65Zr35 alloy in glassy and crystalline states are suggested to play a decisive role in increasing its bulk-glass-forming ability.

MM 65.6 Thu 18:30 H26

Structure formation in binary amorphous Al alloys with early transition metals from the 4th, 5th, and 6th period — •Martin Stiehler[1], Danny Müller[2], Michael Pleul[1], and Peter Häussler[1] — [1]Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]now at Roth & Rau AG, 09337 Hohenstein-Ernstthal, Germany

Amorphous phases as precursors of the crystalline state are indispensable model systems to study 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 between the global subsystems of the electrons on the one hand and the static structure on the other hand. Especially for binary Al-TM alloys (TM: the transition metals of the 4th period Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu) we already reported on an electronic influence on phase stability involving hybridization effects between the Al-p- and the TM-d-states.

In this contribution we report on an extension of these investigations to systems with transition metals of the 5th and 6th period. Especially, we will present results on structural and electronic properties of the binary systems Al-(Sc,Y,La,Ce) in the amorphous state. Although the four systems contain early transition metals from three different periods of the periodic table, they exhibit very similar properties, seemingly related to a mean valency of 1,5e/a in terms of the resonance model.

MM 65.7 Thu 18:45 H26

On structural and electronic properties of Al-Pd Alloys — •Pierre Pudwell, Nan Jiang, and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

In recent years we reported on an electronic influence on phase stability of Al-3d-TM alloys (TM: Sc, ..., Cu). The electronic influence is based on an internal exchange of momentum between global subsystems, namely the electronic system and the forming static structure. Both systems come into resonance to each other. The resonance is enhanced by hybridization effects between Al-p- and TM-d-states. Structure formation, phase stability and the evolution of electronic transport properties were found to be strongly related. In order to test whether such a hybridization enhanced resonance is also effective in other systems, we are about to extend our investigations to systems with 4d- and 5d-TM.

In our contribution we show data on Al-Pd alloys as representative for a system with 4d-TM. Thin films of the material were deposited insitu at about 4K, the resistivity was measured during annealing from 4K to several hundred K, the static atomic structure after annealing to 350K. By comparing the diameter of the strongest diffraction ring with the diameter of the Fermi-sphere, stabilizing resonances were detected, indicating regions with different structural and electronic properties. Between 30 and 70 at.% Pd, there seems to be a hybridization effect like in the Al-3d-TM sytems. For higher and lower Pd concentrations a resonance effect without hybridization seems to dominate – comparable to simple amorphous alloys without transition metals.