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Overview of Invited Talks and Sessions

(lecture rooms IFW A, IFW B, and IFW D; Poster P5)

Invited Talks

MM 1.1	Mon	10:15–10:45	IFW A	**The physics of nano-carbons explored by atomic resolution transmission electron microscopy** — •Jannik Meyer, Simon Kurasch, Ute Kaiser, Andrey Chuvilin, Gerardo Algara-Siller, Hye-Jin Park, Viera Skakalova, Siegmar Roth, Cristina Gomez-Navarro, Ravi Sundaram, Marko Burghard, Klaus Kern, Jurgen Smet, Takayuki Iwasaki, Ulrich Starke, Jani Kotakoski, Arkady Krasheninnikov
MM 5.1	Mon	14:00–14:30	IFW A	**In situ transmission electron microscopy of growth processes and chemical reactions** — Takeshi Kasama, Jörg R. Jinschek, Thomas W. Hansen, Jakob B. Wagner, Zi-An Li, Michael Farle, •Rafal E. Dunin-Borkowski
MM 13.1	Tue	10:15–10:45	IFW A	**Plasticity in confined volumes: new insights into small-scale plasticity** — •Christian Motz
MM 20.1	Wed	10:15–10:45	IFW A	**Atomic-scale modeling of dislocations in iron** — •Matous Mrovec
MM 24.1	Wed	14:00–14:30	IFW A	**Statistical thermodynamics of defects and interfaces in metals** — •Michael W. Finnis
MM 32.1	Thu	10:15–10:45	IFW A	**Direct simulation of in-situ real time X-ray solidification experiment** — •Charles-André Gandin, Guillaume Reinhart, Nathalie Mangelinck-Noël, Henri Nguyen-Thi, Bernard Billia, José Baruchel

Sessions

MM 1.1–1.1	Mon	10:15–10:45	IFW A	**HV Meyer**
MM 2.1–2.6	Mon	11:00–13:00	IFW A	**Topical Session TEM I**
MM 3.1–3.8	Mon	11:00–13:00	IFW B	**Computational Materials Modelling I**
MM 4.1–4.8	Mon	11:00–13:00	IFW D	**Liquid and Amorphous Metals I**
MM 5.1–5.1	Mon	14:00–14:30	IFW A	**HV Dunin-Borkowski**
MM 6.1–6.3	Mon	14:30–15:30	IFW A	**Topical Session TEM II**
MM 7.1–7.4	Mon	14:30–15:30	IFW B	**Computational Materials Modelling II**
MM 8.1–8.4	Mon	14:30–15:30	IFW D	**Liquid and Amorphous Metals II**
MM 9.1–9.5	Mon	15:45–17:30	IFW A	**Topical Session TEM III**
MM 10.1–10.7	Mon	15:45–17:30	IFW B	**Computational Materials Modelling III**
MM 11.1–11.6	Mon	15:45–17:15	IFW D	**Liquid and Amorphous Metals III**
MM 12.1–12.53	Mon	17:30–19:00	P5	**Postersitzung I**
MM 13.1–13.1	Tue	10:15–10:45	IFW A	**HV Motz**
MM 14.1–14.6	Tue	11:00–13:00	IFW A	**Topical Session TEM IV**
MM 15.1–15.8	Tue	11:00–13:00	IFW B	**Computational Materials Modelling IV**
MM 16.1–16.8	Tue	11:00–13:00	IFW D	**Structural Materials**
MM 17.1–17.5	Tue	14:00–15:30	IFW A	**Topical Session TEM V**
MM 18.1–18.6	Tue	14:00–15:30	IFW B	**Mechanical Properties I**
MM 19.1–19.6	Tue	14:00–15:30	IFW D	**Transport**

MM 20.1–20.1	Wed	10:15–10:45	IFW A	**HV Mrovec**
MM 21.1–21.5	Wed	11:00–13:00	IFW A	**Topical Session Electron Theory I**
MM 22.1–22.6	Wed	11:00–13:00	IFW B	**Topical Session TEM VI**
MM 23.1–23.9	Wed	11:00–13:15	IFW D	**Phase Transformations I**
MM 24.1–24.1	Wed	14:00–14:30	IFW A	**HV Finnis**
MM 25.1–25.3	Wed	14:30–15:30	IFW A	**Topical Session Electron Theory II**
MM 26.1–26.3	Wed	14:30–15:30	IFW B	**Topical Session TEM VII**
MM 27.1–27.5	Wed	14:30–15:45	IFW D	**Phase Transformations II**
MM 28.1–28.5	Wed	15:45–17:15	IFW A	**Topical Session Electron Theory III**
MM 29.1–29.5	Wed	15:45–17:00	IFW B	**Topical Session TEM VIII**
MM 30.1–30.4	Wed	16:15–17:15	IFW D	**Complex Materials**
MM 31.1–31.54	Wed	17:15–18:45	P5	**Postersitzung II**
MM 32.1–32.1	Thu	10:15–10:45	IFW A	**HV Gandin**
MM 33.1–33.5	Thu	11:00–13:00	IFW A	**Topical Session Electron Theory IV**
MM 34.1–34.8	Thu	11:00–13:00	IFW B	**Nanomaterials I**
MM 35.1–35.7	Thu	11:00–13:00	IFW D	**Topical Session Heterogeneous Nucleation I**
MM 36.1–36.6	Thu	14:00–16:00	IFW A	**Topical Session Electron Theory V**
MM 37.1–37.8	Thu	14:00–16:00	IFW B	**Nanomaterials II**
MM 38.1–38.6	Thu	14:00–16:00	IFW D	**Topical Session Diffussionless Transformations I**
MM 39.1–39.11	Thu	16:15–19:00	IFW A	**Computational Materials Modelling V**
MM 40.1–40.5	Thu	16:15–17:30	IFW B	**Nanomaterials III**
MM 41.1–41.6	Thu	16:15–17:45	IFW D	**Topical Session Diffussionless Transformations II**
MM 42.1–42.5	Thu	17:45–19:00	IFW B	**Functional Materials I**
MM 43.1–43.4	Thu	18:00–19:00	IFW D	**Mechanical Properties II**
MM 44.1–44.11	Fri	10:30–13:15	IFW A	**Functional Materials II**
MM 45.1–45.5	Fri	10:30–11:45	IFW B	**Topical Session Heterogeneous Nucleation II**
MM 46.1–46.11	Fri	10:30–13:15	IFW D	**Mechanical Properties III**

Topical Sessions "New Developments in Transmission Electron Microscopy of Materials"

Organizers: Erdmann Spiecker (Universität Erlangen-Nürnberg), Knut W. Urban (Research Centre Juelich GmbH)
Over the past decade remarkable progress has been achieved in various fields of transmission electron microscopy (TEM). Advances in instrumentation, like aberration correction, new electron sources, improved energy filters and fast detector systems, have not only pushed the limits of spatial and energy resolution to values hardly conceivable before. Novel types of experiments have become feasible, e.g. in the fields of 3D analysis and in-situ microscopy, supported by new tools and techniques for TEM sample preparation and manipulation. The way TEM can contribute not only to a structural characterization of materials and nanostructures but also to a deeper understanding of their properties and processes is more and more recognized and appreciated. The goal of the symposium is to bring together and stimulate discussion among researchers from various disciplines (materials science, physics, chemistry, mineralogy) who develop or apply advanced TEM techniques in their research.

Topical Sessions "Electron Theory in metal physics- magnetic materials, thermodynamics and kinetics of structural defects"

Organizers: Ralf Drautz (Ruhr-Universität Bochum), Christian Elsässer (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg), Bernd Meyer (Friedrich-Alexander-Universität Erlangen-Nürnberg)
Density functional theory (DFT) has been established as a reliable and transferable method for the quantitative atomic-level simulation of properties of materials. Simplified models that are derived or parameterized from DFT allow to establish frameworks for modelling properties of materials on coarser levels. With this symposium we encourage metal physicists, theoreticians and experimentalists, to highlight the importance of simplified descriptions of the electronic structure for the development of physical models of metallic materials. The symposium will be dedicated to Manfred Fähnle on the occasion of his 60th birthday. It will focus on four main topics, represented by invited lectures of prominent researchers, as follows:

- Electron theory for metals - applications and recent developments
- Magnetism and spin dynamics in metals
- Intermetallic phases and cluster expansions
- Thermodynamics and kinetics of structural defects

Topical Sessions "Heterogeneous Nucleation and Microstructure Formation: Steps towards a system- and scale-bridging understanding"

Organizers: Heike Emmerich (Universität Bayreuth), Gerhard Wilde (Universität Münster)
A detailed understanding of heterogeneous nucleation is still regarded as one of the open issues of solidification despite the number of classical theories available to describe it at different levels. Lately, a combination of new advanced experimental approaches jointly with molecular and thermodynamic modelling, as well as phase-field simulations, has been proven to provide an efficiently synergetic interplay which helps to access new aspects of heterogeneous nucleation and initial microstructure formation and which enhances the understanding of the basic underlying mechanisms. This session is devoted to investigations in this field with either theoretical, experimental or simulation methods.

Topical Sessions "Diffussionless transformations in magnetic and ferroelectric bulk and thin films"

Organizers: Sebastian Fähler (IFW Dresden), Dietrich Hesse (Max-Planck-Institut für Mikrostrukturphysik, Halle)
Diffusionless phase transformations are at the core of functional materials as (magnetic) shape memory alloys, ferroelectrics, caloric and multiferroic materials. These phase transformations can be controlled by external electric or magnetic fields as well as stress and pressure. Hence these complex materials exhibit multiple new physical effects, which are currently examined with dedicated theoretical and experimental methods.
By highlighting the close connections between the different classes of functional materials this symposium brings together different communities. As external constraints significantly affect these transformations, in particular thin films and nanostructures helped to understand the underlying coupling mechanism.

Invited talks of the joint SKM-Symposium "Diffusionless Transformations in Magnetic and Ferroelectric Bulk and Thin Films" (SKM-SYDT)

See SKM-SYDT for the full program of the symposium.

SKM-SYDT 1.1	Thu	10:30–11:00	TRE Ma	**Domain boundaries as active elements in multiferroics and martensites: steps towards Domain Boundary Engineering** — •Ekhard K.H. Salje
SKM-SYDT 1.2	Thu	11:00–11:30	TRE Ma	**Intermediate Phases in Perovskite Solid Solutions** — •Ian Reaney, Clive Randall, David Woodward
SKM-SYDT 1.3	Thu	11:30–12:00	TRE Ma	**Adaptive martensite and giant strain effects in multiferroics** — •Ulrich K. Rössler
SKM-SYDT 1.4	Thu	12:00–12:30	TRE Ma	**Nature of magnetic coupling in Ni-Mn-based martensitic Heusler alloys** — •Mehmet Acet, Seda Aksoy, Eberhard F. Wassermann, Lluis Manosa, Antoni Planes
SKM-SYDT 1.5	Thu	12:30–13:00	TRE Ma	**Orthorhombic to tetragonal transition of $SrRuO_3$ layers in $Pr_{0.7}Ca_{0.3}MnO_3/SrRuO_3$ superlattices** — •Michael Ziese, Francis Bern, Ionela Vrejoiu, Eckhard Pippel, Elizaveta Nikulina

Invited talks of the joint SKM-Symposium "SKM-Symposium Heterogenous Nucleation and Microstructure Formation: Steps towards a System- and Scale-bridging Understanding" (SKM-SYMF)

See SKM-SYMF for the full program of the symposium.

SKM-SYMF 1.1	Thu	14:30–15:00	TRE Ma	**Visualizing the structural solid-liquid transition with colloidal suspensions** — •Peter Schall
SKM-SYMF 1.2	Thu	15:00–15:30	TRE Ma	**Crystallization process in suspensions of hard spheres** — •Tanja Schilling, Hans-Joachim Schoepe, Martin Oettel, George Opletal, Ian Snook
SKM-SYMF 1.3	Thu	15:30–16:00	TRE Ma	**Homogeneous bulk, surface, and edge nucleation in crystalline nanodroplets** — •Kari Dalnoki-Veress, Jessica Carvalho
SKM-SYMF 1.4	Thu	16:00–16:30	TRE Ma	**Polymer Crystallization: Ordered Structures in Complex Systems** — •Jens-Uwe Sommer
SKM-SYMF 1.5	Thu	16:30–17:00	TRE Ma	**Phase formation and microstructure development in multicomponent alloys** — •Jürgen Eckert

Annual General Meeting of the Metal and Material Physics Division

Mittwoch 19:00 - 20:00 IFW B

- Report of the chairman of the Metal and Material Physics Division
- Invited talks and symposia for the next spring meeting 2012
- Other topics

MM 1: HV Meyer

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

Invited Talk MM 1.1 Mon 10:15 IFW A

The physics of nano-carbons explored by atomic resolution transmission electron microscopy — •Jannik Meyer[1,2], Simon Kurasch[2], Ute Kaiser[2], Andrey Chuvilin[2], Gerardo Algara-Siller[2], Hye-Jin Park[3], Viera Skakalova[3], Siegmar Roth[3], Cristina Gomez-Navarro[3], Ravi Sundaram[3], Marko Burghard[3], Klaus Kern[3], Jurgen Smet[3], Takayuki Iwasaki[3], Ulrich Starke[3], Jani Kotakoski[4], and Arkady Krasheninnikov[4] — [1]University of Vienna, Department of Physics, Vienna, Austria — [2]University of Ulm, Germany — [3]Max Planck Institute for solid state physics, Stuttgart, Germany — [4]University of Helsinki, Finland

Graphene is an outstanding new material that promises a wide range of new applications and scientific insights, and it is closely related to carbon nanotubes, fullerenes or graphite. Hence, the graphene structure and its defects are of outstanding interest for the science and applications of these new materials. Static deformations, topological defects, various vacancy configurations or the two-dimensional equivalent of dislocations were studied by aberration-corrected transmission electron microscopy (TEM). Existing defects in as-synthesized CVD graphene and reduced graphene oxide were analyzed. The formation and evolution of defects under electron irradiation is observed in real time with atomic resolution. High-energy electron irradiation provides a "randomization" of some atoms, which then allows new insights into the complicated bonding behaviour in carbon materials. Further, we show that the charge distribution in graphene defects or other 2-D materials can be analyzed on the basis of high-resolution TEM images.

MM 2: Topical Session TEM I

Time: Monday 11:00–13:00 Location: IFW A

Topical Talk MM 2.1 Mon 11:00 IFW A

Study at picometres precision of structure and properties of oxide ferroelectrics — •Chun-Lin Jia — Institute of Solid State Research and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Epitaxial thin films of ferroelectric oxides have attracted increasingly intensive research both for fundamental and application issues. The physical properties of these film systems depend strongly on the particular microstructure and configuration of lattice defects.

By means of a spherical aberration corrector in a transmission electron microscope the value of the spherical aberration Cs can be tuned to negative values resulting in a novel imaging technique: The negative Cs imaging (NCSI) technique. The images obtained with the NCSI technique are superior to positive Cs images in the magnitude of the contrast and the image intensity of atom columns. The image signal obtained with the NCSI technique is significantly more robust against noise, resulting in measurement of atomic positions with a precision of a few picometres.

In this talk, we present the results of a study using NCSI technique of the epitaxial thin-film system of PbZr0.2Ti0.8O3. The positions of all the atomic species are measured, unit cell by unit cell, with a precision of a few picometres. On this basis the relative ion displacements in the individual unit cells are calculated. These displacements depict the details of electric dipole moments in domains, at domain walls, as well as at defect area.

Topical Talk MM 2.2 Mon 11:30 IFW A

In-situ TEM as a nanolab for studying electrical and electrochemical transport mechanisms in perovskites — •Christian Jooss[1], Jonas Norpoth[1], Stephanie Raabe[1], Malte Scherff[1], Joerg Hoffmann[1], James Ciston[2], Dong Su[2], Lijun Wu[2], and Yimei Zhu[2] — [1]Institute of Materials Physics, University of Goettingen, Germany — [2]Brookhaven National Laboratory, Upton NY, USA

Perovskite oxide materials with strong electronic or electron-lattice correlations exhibit a rich variety of properties ranging from colossal resistance effects over remanent resistance switching to multi-electron transfer in catalytic reactions. Intrinsic inhomogeneities such as electronic phase separation on the nanoscale and extreme sensitivity to defect structure make atomic resolution studies of properties and behavior in external fields highly desirable, in order to understand underlying mechanisms. In this talk, we will show through two examples, the opportunities of in-situ TEM for a detailed understanding of electrical transport properties in doped manganites. In one example, a piezo-controlled STM tip (Nanofactory) has been used to electrically stimulate a hole-doped manganites and metal-manganites heterostructures. The induced resistance change was correlated to the locally induced structural and electronic changes. In the second example, in-situ studies of water splitting using $CaMnO_3$ based catalysts have been performed in a FEI Titan microscope with an environmental chamber. Catalytic activity was observed at specific crystalline sites and related changes in the oxidation state of the Mn cations during the reaction were recorded via Electron Energy Loss Spectroscopy.

MM 2.3 Mon 12:00 IFW A

Direct evidence for cation non-stoichiometry and Cottrell atmospheres around dislocation cores in functional perovskite oxide interfaces — •Miryam Arredondo[1], Quentin Ramasse[2], Matthew Weyland[3], Ionela Vrejoiu[1], Dietrich Hesse[1], Nigel Browning[5], and Valanoor Nagarajan[4] — [1]MPI of Microstructure Physics, Halle, Germany — [2]LBNL NCEM, Berkeley, CA, USA. — [3]MCEM, Monash Uni., Victoria, Australia — [4]SMSE, UNSW, Australia — [5]Chem. Eng. & Mater. Sci., UC Davis, USA.

Exploiting the electronic properties of oxides in functional devices requires their deposition on an underlying substrate, often with an unavoidable lattice mismatch. We consider the chemical implications in the accommodation of this mismatch by misfit dislocations, by the characterization of the lattice mismatched system: a PbZr0.52Ti0.48O3 ferroelectric film deposited on a SrRuO3 electrode-buffered SrTiO3 substrate. Cs-corrected Z-contrast imaging and chemical analysis techniques are exploited to yield evidence for cation excess within dislocation cores at the interface. Multislice image simulations reproduces fairly well the observed image contrast. EDX maps reveal Pb and Sr interdifussion and EELS scans at the core reveal that it is oxygen-deficient compared to the defect-free lattice. Geometric phase and theoretical elastic modeling reveal that the local strain around the dislocation core is sufficient to create stress-assisted diffusion of cations. This study provides insights into the link between the local chemistry, physical structure and observed functional behavior in the ferroelectric at the proximity of a dislocation core.

MM 2.4 Mon 12:15 IFW A

Scandate/Titanate Interfaces: Structure and Composition on the Atomic Scale — •Martina Luysberg[1], Jürgen Schubert[2], Kourosh Rahmanizadeh[3], Gustav Bihlmayer[3], Lena Fitting Kourkoutis[4], and David A Muller[4] — [1]Institute of Solid State Research IFF-8 and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Research Centre Jülich, D-52425 Jülich, Germany — [2]Institute of Bio- and Nanosystems and JARA-FIT, Research Centre Jülich, D-52425 Jülich, Germany — [3]Institute of Solid State Research IFF-1, Research Centre Jülich, D-52425 Jülich, Germany — [4]Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA

When scandates and titanates are joint at an interface, a polar discontinuity occurs. Unlike the polar interface between $LaAlO_3$ and $SrTiO_3$, where a conducting interface has been discovered, the scandate-titanate heterojunctions remain electrical insulating. Recently we reported on an intermixing of the cations across the interface of $DyScO_3$ and $SrTiO_3$. This intermixing of ions of different valency counteracts the interface dipoles arising from the polar discontinuity, making the interface insulating. In the paper presented here we focus on an additional property of the interface: an ordered interface structure. High resolution electron microscopy and electron energy loss spectroscopy on individual atomic columns will be shown, which reveal an ordering on the Sr/RE (RE=Gd or Dy) sublattice. These results will be

discussed in conjunction with ab-initio calculations.

MM 2.5 Mon 12:30 IFW A

Electron beam induced surface diffusion on metallic nanoparticles — •Alexander Surrey[1], Darius Pohl[1], Ulrich Wiesenhütter[2], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01156 Dresden, Germany — [2]FZ Dresden, Postfach 510119, D-01314 Dresden, Germany.

The predominant mass transport mechanism during the coalescence of adjacent metallic nanoparticles is assumed to be surface diffusion. Upon exposure to an electron beam in a transmission electron microscope (TEM) the diffusion of surface atoms towards the sintering neck is stimulated thereby reducing the particles's surface free energy. This electron beam induced inter-particle coalescence is investigated in FePt and Au nanoparticles with icosahedral or truncated octahedral structure by means of aberration-corrected TEM. The particles are prepared by inert gas condensation which provides for free and uncovered surfaces. Aberration-corrected TEM is employed to monitor and analyze quantitatively temporal changes of the surface atom configurations on particle facets oriented parallel to the electron beam. It is observed that the path of the surface atoms towards the sintering neck is chosen to always optimize the local coordination. The influence of the electron energy (which can be chosen by adjusting the acceleration voltage) on the beam-induced surface diffusion is discussed.

MM 2.6 Mon 12:45 IFW A

Soot formation in a diesel engine — •Mirza Mačković[1,2], Sebastian Pflaum[3], Gerhard Frank[2], Erdmann Spiecker[1], Georg Wachtmeister[3], and Mathias Göken[1,4] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Cauerstraße 6, 91058 Erlangen, Germany — [2]Institute of Biomaterials, Cauerstraße 6, 91058 Erlangen, Germany — [3]Institute of Combustion Engines, Schragenhofstraße 31, 80992 Munich, Germany — [4]Department of Materials Science and Engineering, General Materials Properties, Martensstraße 5, 91058 Erlangen, Germany

Diesel engine soot is known as one of the main environmental pollutants and has become an important environmental and scientific topic. Diesel soot is a product of pyrolysis or incomplete combustion of hydrocarbons. Especially, the formation mechanism of soot particles is one of the central themes of research activities in the area of combustion and pyrolysis of fossil fuels. It is known that soot particles from the exhaust of diesel engines appear as chain-like agglomerates and consist of several tens to hundreds of primary soot particles. In this study soot particles are collected from nearly the centre of the combustion chamber of a diesel engine, using a newly developed technique, and analyzed by means of transmission electron microscopy and electron energy loss spectroscopy. Thus the development of the soot nanostructure could be shown as a function of crank angle and time after the combustion of the diesel fuel begins. The early formation, growth and oxidation of the soot particles are observed and some aspects regarding the complex process of soot formation are proposed.

MM 3: Computational Materials Modelling I

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

MM 3.1 Mon 11:00 IFW B

Properties of positrons at defects in metal — •Martin Offenberger[1], Hubert Ebert[1], and John Banhart[2] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz Zentrum Berlin

Positron annihilation is a well established tool to study defects in metals in experiment. To simulate positron annihilation experiments, an accurate and efficient description of both positrons and defects is needed. To calculate clusters of impurity atoms in a metal host, we use the Korringa-Kohn-Rostoker Green's function method (KKR-GF). This approach deals with the defect region by means of the Dyson equation instead of a supercell approach, avoiding artificial boundary conditions. Positrons are then calculated according to the conventional scheme suggested e.g. by Boroński and Nieminen. Results of our calculations presented include positron charge distributions, density of states and annihilation lifetimes for a variety of defects in Aluminium. In addition, the properties of defects like vacancies and transition metal impurity-vacancy dimers as positron traps will be discussed.

MM 3.2 Mon 11:15 IFW B

Ab-initio-based prediction of the vacancy concentration in the $Ni_{<50}Al_{50}$ B2 phase — •Tobias C. Kerscher[1], Daniel Lerch[2], Gus L. W. Hart[3], Quinn O. Snell[4], and Stefan Müller[1] — [1]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, 21073 Hamburg, Germany — [2]Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik 2, Staudtstr. 7, 91058 Erlangen, Germany — [3]Brigham Young University, Department of Physics and Astronomy, Provo UT 84602, USA — [4]Brigham Young University, Computer Science Department, Provo UT 84602, USA

The B2 phase of Ni–Al gains its technical importance from the high melting point (1638 °C). Off its ideal 50-50 stoichiometry, this B2 phase is stabilised by the formation of vacancies on the Ni sublattice. We use our code UNCLE [1] to construct an ab-initio-based cluster-expansion Hamiltonian for this ternary (Ni, Al, vacancy) system. Thermodynamic Monte Carlo simulations in the (quasi)grand-canonical ensemble are applied to account for configurational entropy and to predict the equilibrium concentration of the vacancies as a function of temperature. Since point defect concentrations are expected to be in the order of ppm, the correspondingly large Monte Carlo cells are addressed with the help of a recently demonstrated parallel Monte Carlo implementation in UNCLE.

Supported by Deutsche Forschungsgemeinschaft.

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

MM 3.3 Mon 11:30 IFW B

Ab initio determination of diffusion mechanisms in FeAl — •Niko Sandschneider, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

Iron aluminides are a promising material class for industrial high temperature applications. FeAl shows a very high vacancy concentration (several percent at T>1000 K) which severely affects its mechanical properties. It is therefore crucial to understand the generation and diffusion behavior of those vacancies.

The simplest diffusion mechanism which preserves long-range order in B2-FeAl is the next-nearest neighbor (NNN) jump of a vacancy. As a first step we performed ab initio calculations to determine the formation energies of the defects in FeAl. Four defects were investigated, namely vacancies and antisite atoms on the Fe and Al sublattices. We found that the Al vacancy has a large formation energy compared to the other defects. Therefore the NNN jump was only investigated for Fe vacancies. In a second step we calculated the migration barrier of this process using the climbing image nudged elastic band method.

Several more sophisticated mechanisms are proposed in the literature. A very promising candidate is the triple defect mechanism. We also performed nudged elastic band calculations for this mechanism and found a migration barrier which is significantly lower than for the NNN jump and several other diffusion mechanisms. We therefore conclude that the triple defect mechanism is the energetically most favorable diffusion mechanism.

MM 3.4 Mon 11:45 IFW B

Ab-initio and atomistic study of the ferroelectric properties of Cu doped potassium niobate — •Sabine Körbel and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

$KNbO_3$ is one end member of the solid solution $(K, Na)NbO_3$ (KNN), which has promising ferroelectric properties to become a future lead-free substitute for lead zirconate titanate $Pb(Zr, Ti)O_3$ (PZT) in piezoelectric actors and sensors. Both KNN and PZT exhibit a phase transition with composition and a morphotropic phase boundary, at which enhanced piezoelectric coefficients are obtained. The material properties of PZT and KNN are commonly optimized by doping. E.g., CuO can be added when fabricating KNN as a sintering aid. Ab initio density functional theory and atomistic simulation using a classical shell model potential have been combined to investigate low Cu concentrations in the $KNbO_3 - CuNbO_3$ system. The atomistic model predicts a morphotropic phase boundary at a few percent Cu, analoguous to

the one found in the $LiNbO_3 - KNbO_3$ system [1,2].

[1] Y. Guo, K. Kakimoto, and H. Ohsato, Appl. Phys. Lett. **85**, 4121 (2004).
[2] D. I. Bilc and D. J. Singh, Phys. Rev. Lett. **96**, 147602 (2006).

MM 3.5 Mon 12:00 IFW B

Defects in ferrite: from quantum-mechanical calculations to long-range elastic effects — •Alexander Udyansky[1], Johann von Pezold[1], Alexey Dick[1], Vladimir Bugaev[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Interstitial Fe-based solid solutions with a low content of C, N, O, B, C+N and H impurities have been studied by combining first principles simulations with the reciprocal space microscopic elasticity theory (MET). This approach allows for a highly efficient description of long-range elastic interactions, which generally control interstitial-interstitial interactions. The short-range chemical interactions, as well as the parameters entering the MET are obtained by density functional theory (DFT) in the generalized gradient approximation, using rather modest supercell sizes. The proposed approach provides a direct insight into the formation mechanism of martensite and its stability limit. For example, tetragonal states are predicted to be preferred even at low impurity concentrations due to a thermodynamically driven orientational ordering of impurities. Furthermore we were able to predict the low impurity concentration part of Fe-based solid solutions phase diagrams and its dependence on the local strain state of the system. Finally, the impurity content is found to strongly affect the vacancy concentration within the host matrix.

MM 3.6 Mon 12:15 IFW B

Ab initio study of effect of non-magnetic impurities on the structure and properties of grain boundaries and free surfaces in nickel — •Monika Všianská[1,2] and Mojmír Šob[1,2] — [1]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [2]Istitute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

We have studied segregation of sp-elements of the 3rd, 4th and 5th period (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at the $\Sigma5(210)$ grain boundary (GB) and (210) free surface (FS) in fcc nickel. We analysed the geometric configuration and the distribution of magnetic moments at the GB and FS without and with impurities. Whereas there is a slight enhancement of magnetization at the clean GB with respect to bulk nickel, the studied impurities entirely kill or strongly reduce ferromagnetism at the GB and its neighbourhood. We also determined the embrittling energy and its chemical and mechanical part from the difference between the GB and FS binding energies on the basis of the Rice-Wang model. We predict interstitially segregated Si as a GB cohesion enhancer, substitutionally segregated Al and interstitially segregated P with none or minimal strengthening effect and interstitially segregated S, Ge, As, Se and substitutionally segregated Ga, In, Sn, Sb and Te as GB embrittlers in Ni.

MM 3.7 Mon 12:30 IFW B

Ab initio study of energetics and magnetism of Fe, Co and Ni along the trigonal deformation path — Martin Zelený[1], Martin Friák[2,3], and •Mojmir Šob[4,1] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Max-Planck Institut für Eisenforschung, GmbH, Düsseldorf, Germany — [3]Institute of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have calculated total energies of iron, cobalt and nickel in several magnetic phases as a function of atomic volume and trigonal deformation and found the phase boundaries between various magnetic modifications in Fe and Ni. In case of Ni, these phase boundaries occur even at the experimental atomic volume. On the other hand, Co keeps its ferromagnetic order in the whole region of the volume and shape deformation studied. Fe does not exhibit any transition between the ferromagnetic and non-magnetic arrangement, but at low atomic volumes around the fcc structure, phase boundaries between the ferromagnetic high-spin, ferromagnetic low-spin and antiferromagnetic states have been found.

MM 3.8 Mon 12:45 IFW B

Point-defect-mediated dehydrogenation of alane — •Lars Ismer, Anderson Janotti, and Chris G Van de Walle — University of California at Santa Barbara, CA 93106, United States

For the engineering of better hydrogen storage materials a systematic understanding of their hydrogen sorption kinetics is crucial. We present a systematic analysis of the dehydrogenation kinetics of alane (AlH3), one of the prime candidate materials for hydrogen storage. Using hybrid-density functional calculations we determine the concentrations and mobilities of point defects and their complexes. Kinetic Monte Carlo simulations are used to describe the full dehydrogenation reaction. We show that under dehydrogenation conditions charged hydrogen vacancy defects form in the crystal, which have a strong tendency towards clustering. The vacancy clusters denote local nuclei of Al phase, and the growth of these nuclei eventually drives the AlH3/Al transformation. However, the low concentration of vacancy defects limits the transport of hydrogen across the bulk, and hence acts as the rate-limiting part of the process. The dehydrogenation is therefore essentially inactive at room temperature, explaining why AlH3 is metastable for years, even though it is thermodynamically unstable. Our derived activation energy and dehydrogenation curves are in excellent agreement with the experimental data, providing evidence for the relevance of bulk point-defect kinetics. Based on our results we argue that manipulating vacancy defect concentrations, e.g., by the usage of irradiation, will allow control over hydrogen sorption kinetics, opening up new engineering strategies.

MM 4: Liquid and Amorphous Metals I

Time: Monday 11:00–13:00 Location: IFW D

MM 4.1 Mon 11:00 IFW D

Effects of rhenium on glass formation and mechanical properties of metastable ZrCuAl alloys — •Steffen Schmitz, Wolfgang Löser, Hansjörg Klauss, Christine Mickel, and Bernd Büchner — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

The effect of small additives of Re on a metallic glass forming alloy $(Cu_{46}Zr_{46}Al_8)_{100-x}Re_x$ (x = 1, 2) was investigated for samples of different sizes. Re possess a positive enthalpy of mixing within the Cu-Re terminal system. Splat quenched foils of ≈ 40 μm thickness display amorphous structure. Their crystallization temperature increases from $T_x = 500$ to 510 °C with increasing Re fraction at nearly constant glass formation temperature $T_g = 440$ °C. By contrast, injection cast rods consist of B2 - CuZr type metastable phase dendrites, a cubic CuZrAl type phase and randomly distributed small particles of a Re-rich phase. The presence of metastable phases leads to a unique combination of mechanical properties of as-cast rods which display high strength at sizeable plastic deformation up to $\epsilon_p \approx 4\,\%$ and an extended range of work hardening prior to failure.

MM 4.2 Mon 11:15 IFW D

Study of mechanical property and crystallization of a Zr-CoAl bulk metallic glass — •Jun Tan[1,2,3], Yue Zhang[1], Mihai Stoica[1], Norbert Mattern[1], Fusheng Pan[2], and Jürgen Eckert[1,3] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 27 01 16, D-01171 Dresden, Germany — [2]Materials Science & Engineering College, Chongqing University, 400030 Chongqing, China — [3]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The mechanical property of Zr56Co28Al16 bulk metallic glasses (BMGs) under compression test at room temperature was investigated. The alloy exhibited high fracture strength of approximately 2136 MPa and a pronounced plastic strain of 10.2%. No strainhardening behavior was observed. The evolution of the morphology of the shear bands on the lateral surface of the as-cast samples was studied using scanning electron microscopy (SEM). The plasticity can be attributed to the formation and interaction of multiple shear bands during deforma-

tion. The crystallization behavior was studied by differential scanning calorimetry (DSC) at different heating rates.The crystallization behavior research of this alloy indicates that the precipitation of the B2-ZrCo phase may be further utilized to promote the ductility of the ZrCoAl BMG composites.

MM 4.3 Mon 11:30 IFW D

Inhomogeneous deformartion of metallic glasses — •Stefan Küchemann, Dennis Bedorf, Walter Arnold, and Konrad Samwer — 1. Physikalisches Institut, Universität Göttingen, Germany

Despite recent progress it is still not clear how local rearrangements take place in bulk metallic glasses under external stress. Previous results show that homogeneous deformation can be separated into reversible and irreversible processes which can be interpreted in the potential energy landscape picture.[1]

In the experiments reported in this contribution, we investigated anelasticity in bulk metallic glasses with nominal composition $Pd_{40}Ni_{40}P_{20}$. To modify the potential energy state, structurally relaxed samples were deformed at room temperature. The stresses cover the range from elastic response to inhomogeneous flow. In DSC measurements we found that the heat flow below T_G showed a clear indication for a strain dependence. Thus a certain amount of energy could be stored and is thermally relaxed below T_G.

Financial support by the DFG SFB 602 and the Leibniz-Program is thankfully acknowledged.

[1] J. S. Harmon, M. D. Demetriou, W. L. Johnson, K. Samwer, Anelastic to Plastic Transition in Metallic Glass Forming-Liquids, Phys. Rev. Lett. 99, 135502 (2007)

MM 4.4 Mon 11:45 IFW D

Structure conserving correlation and the Kohlrausch-Williams-Watts relaxation in simulated metallic-glass forming Ni0.5Zr0.5 — •Helmar Teichler — Institut f. Materialphysik, Univ. Göttingen

In glass forming melts near the glass temperature, the alpha-decay reflects relaxation processes with Kohlrausch-Williams-Watts behaviour on macroscopic time scales. Microscopic explanation of these fundamental features is a challenging open question, which needs to understand emergence of slow relaxation with non-exponential response from atomic motions in the melt. Regarding this, we here present an analysis of molecular dynamics simulation results for glass forming Ni0.5Zr0.5. In detail it is shown that (a) the fraction of weakly effective particles (WEPs, in essence the immobile, vibrating atoms) determines the alpha-decay of the incoherent intermittent scattering function (ISF), (b) the WEPs exhibit strong temporal correlations in the way that particles acting as WEPs in an initial time window tend to act as WEPs also at later times, (c) this correlation makes that the alpha-process shows KWW-relaxation while uncorrelated change of particles between immobile and mobile behaviour yields Debye-relaxation.

MM 4.5 Mon 12:00 IFW D

Local mechanical spectroscopy on confined structures of metallic glasses — •Dennis Bedorf, Bo Zhang, Hannes Wagner, Moritz Schwabe, Walter Arnold, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen,Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Our aim is to investigate the local heterogeneity of glasses with an experimental approach. Up to now most of the knowledge about dynamical heterogeneities, like shear-transformation zones or string-like rearrangements, is based on computer studies. An atomic force based method which exploits contact-resonances of the cantilever, also called AFAM [1], enables us to study the elastic response and also anelastic losses on the nm-scale. Recent results have revealed a broad distribution of local moduli for amorphous PdCuSi on this length scale. Motivated by these findings we adopt this method to study size effects in glasses using nanoscaled samples prepared by lithography. First results indicate a significant softening for smaller samples.

[1] M. Kopycinska-Müller, and W. Arnold et al, Z. Phys. Chem. 222, 471 (2008)

MM 4.6 Mon 12:15 IFW D

Microstructure and magnetic properties of Gd-Hf-Co-Al glassy alloys by liquid-liquid phase separation — •Junhee Han[1,2], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [2]TU Dresden, Institute of Materials Science, Dresden, Germany

Phase separated glassy ribbons were prepared in the Gd-Hf-Co-Al system by rapid quenching of the melt. From the Gd55Co25Al20 ternary good glass former, we substitute Gd with Hf by 10, 20, 27.5, 35, 45 and 55 at. %. Due to the strong positive enthalpy of mixing between the principal elements Gd and Hf (ΔHmix = +11kJ/mole) a heterogeneous microstructure is formed consisting of two amorphous phases Gd-enriched and Hf-enriched. For the alloys with clearly phase separated microstructure, nano-meter scale (~100nm) secondary phase separation is observed in each amorphous phase. In the case of the Gd27.5Hf27.5Co25Al20 alloy, coexistence of two different types of microstructure such as a droplet-like and interconnected structure were observed from the areas having different cooling rate. This microstructure evolution is in good agreement with calculation results by Lattice Boltzmann method. On the other hand, measured magnetic properties show the composition and volume fraction dependence of magnetization and transition temperature (Tc) of Gd-Hf-Co-Al system. The saturation magnetization decreases as a function of Hf contents and can be described by a simple mixture model.

[1] A. J. Wagner and J. M. Yeomans, Phys. Rev. Lett., 80 (1998) 1429

MM 4.7 Mon 12:30 IFW D

Influence of initial temperature and cooling rate on the liquid and amorphous structure of Cu47.5Zr47.5Al5 alloy simulated by molecular dynamics — •Valentin Kokotin and Jürgen Eckert — IFW Dresden, Institute for Complex Materials, Postfach 27 01 16, D-01171 Dresden, Germany

Atomic structure in liquid and supercooled/amorphous states has been investigated for the model alloy, Cu47.5Zr47.5Al5, with the help of classical molecular dynamics computer simulations. By rapid quenching from the melt (used initial temperatures: 1200 and 2000 K) at various cooling rates (comprising 6 orders of magnitude), differently relaxed amorphous structures have been prepared. The cooling rate affects the structural and thermodynamic properties significantly. Density and fraction of icosahedra depend exponentially on the cooling rate. The initial temperature of the liquid has rather a tangential influence on the final amorphous structure. The major differences in supercooled structure arise at temperatures below 900K (undercooling of about 300K), where nearly amorphous structure is "born".

MM 4.8 Mon 12:45 IFW D

Magnetocaloric effect of $Fe_{86-x}B_{14}Nb_x$ metallic glasses — •Anja Waske, Björn Schwarz, Norbert Mattern, and Jürgen Eckert — Institut für Festkörper- und Werkstoffforschung (IFW), Dresden

Materials exhibiting the magneto-caloric effect could one day be the basis of a new magnetic cooling concept for consumer use, replacing conventional refrigeration technology. However, currently known materials with high magnetic entropy changes are very expensive and can hence not be applied on mass production scale. Here, we report on the magneto-caloric effect in comparatively cheap Fe-based metallic glasses. Glassy $Fe_{86-x}B_{14}Nb_x$ ribbons were prepared by rapidly quenching the liquid using the melt spinning technique. By diluting the magnetic lattice with Nb dopants, the Curie temperature decreases and, at highest Nb content, approaches room temperature. However, this effect is accompanied by a decrease of the saturation magnetization. From temperature dependent magnetization measurements the magnetic entropy change was calculated using the thermodynamic Maxwell equations. We will present the experimental results as a function of Nb content and discuss the applicability of the material for cooling purposes.

MM 5: HV Dunin-Borkowski

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

Invited Talk MM 5.1 Mon 14:00 IFW A

In situ transmission electron microscopy of growth processes and chemical reactions — Takeshi Kasama[1], Jörg R. Jinschek[2], Thomas W. Hansen[1], Jakob B. Wagner[1], Zi-An Li[3], Michael Farle[3], and •Rafal E. Dunin-Borkowski[1] — [1]Center for Electron Nanoscopy, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [2]FEI Europe, Achtseweg Noord 5, 5600 KA Eindhoven, The Netherlands — [3]Universität Duisburg-Essen, Lotharstr.1, 47048 Duisburg, Germany

Modern environmental transmission electron microscopes (ETEMs) can be equipped with aberration correctors and monochromators to improve spatial resolution and spectral sensitivity during dynamic studies of chemical reactions and growth processes. We have recently installed an FEI Titan 80-300 ETEM, in which seven different gases can be introduced into the microscope at pressures of up to 1500 Pa and additional gases can be connected when required. As a model system, we have chosen to study Au nanoparticles on BN, graphene and silica supports in oxidizing and reducing environments at elevated temperature. The particles are observed to sinter both by migration and coalescence and by Ostwald ripening, with different sintering mechanisms occurring simultaneously. We have also recently used ETEM to study the reduction of single crystalline 15 nm Fe oxide cubes to Fe at elevated temperature in hydrogen in the electron microscope, and their subsequent reoxidation to polycrystalline Fe oxide in the electron beam. I will discuss the degree to which both sets of experiments may be affected by ionization of the gas and charging of the specimen.

MM 6: Topical Session TEM II

Time: Monday 14:30–15:30 Location: IFW A

Topical Talk MM 6.1 Mon 14:30 IFW A

Excitation of Surface Plasmon Resonances in Metallic Nanostructures — •Peter van Aken[1], Wilfried Sigle[1], Burcu Ögüt[1], Nahid Talebi[1,2], Christoph Koch[1], and Ralf Vogelgesang[3] — [1]Stuttgart Center for Electron Microscopy, Stuttgart, Germany — [2]Photonics Research Laboratory, University of Tehran, Iran — [3]Max-Planck-Institute for Solid State Research, Stuttgart, Germany

In this contribution, the dielectric responses of metallic particles, like triangular Ag nanoprisms, of nanoholes and of rectangular slits in thin Ag films, drilled by using a focused ion beam, are studied by acquiring energy-filtering transmission electron microscopy (EFTEM) series on a 2k x 2k CCD camera using a 0.2 eV energy selecting slit for both the monochromator and the imaging energy filter with an acquisition time between 20 s and 30 s per image using the Zeiss SESAM microscope. We map surface plasmon resonances (SPRs) at optical wavelengths on single triangular silver nanoprisms, where extra multipolar SPRs on these nanoparticles could be detected. EFTEM images from the nanoholes in a thin Ag film were obtained at energy losses in the range from 0.6 eV to 2.8 eV. We observe localized SPRs as very pronounced intensity maxima visible in the image series. The length scale of some features is as small as 10-20 nm which can presently not be imaged by other besides electron microscopy techniques. We find two resonances that are typical for single, isolated holes. A comparison with calculations based on the discrete dipole approximation (DDSCAT) shows that these are dipolar and quadrupolar resonances.

MM 6.2 Mon 15:00 IFW A

Aberration-corrected imaging of binary metal nanoparticles — •Darius Pohl, Björn Bieniek, Elias Mohn, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, Helmholtzstr. 20, D-01156 Dresden, Germany.

Aberration-corrected high resolution transmission electron microscopy (HRTEM) is used to study the lattice structure of single crystalline FePt and FeNi nanoparticles. Due to the delocalization-free imaging a direct and precise measurement of atom positions and lattice constants even at the very surface layers becomes feasible. For a wide range of particle sizes and morphologies, metallic nanoparticles of binary alloys are found to show an expansion of the lattice in the surface layers. In order to gain insight into the origin of the observed surface-near lattice expansion, molecular dynamics (MD) simulations were performed. A comparison of the experimental HRTEM images with the relaxed model structures clearly reveals that segregation phenomena are responsible for the dilated lattice at the particle surface.

In order to investigate the influence of oxygen on the surface-near lattice expansion, oxidation sensitive systems need to be investigated. Since FeNi is less noble and thus more susceptible to oxidation than FePt, the effect of structural changes due to oxidation should be much more pronounced in the former. From a comparison of un-oxidized and oxidized FeNi nanoparticles, the influence of oxygen on the surface-near lattice constant of the metallic particle core is determined to be almost negligible.

MM 6.3 Mon 15:15 IFW A

Metadislocations in Complex Metallic Alloys: A High-Resolution Scanning Transmission Electron Microscopy Study — •Marc Heggen, Lothar Houben, and Michael Feuerbacher — Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Juelich GmbH, D-52425 Juelich, Germany

Metadislocations are highly complex defects which involve several hundreds of atoms in their core. We present a microstructural investigation on Metadislocations using aberration-corrected high-resolution scanning transmission electron microscopy. A novel and highly complex deformation mechanism is found which is based on the movement of a metadislocation core mediating strain and separate escort defects [1]. Upon deformation, the escort defects move along with the metadislocation core and locally transform the material structure. This mechanism implies the coordinated movement of hundreds of atoms per elementary step. Although the mechanism is very complex, it can be described by a simple jigsaw-puzzle-like rearrangement of basic structural subunits.

[1] M. Heggen, L. Houben, M. Feuerbacher, Nature Materials 9 (2010) 332.

MM 7: Computational Materials Modelling II

Time: Monday 14:30–15:30 Location: IFW B

MM 7.1 Mon 14:30 IFW B

Alkane Adsorption in Chabazite - Different Ways to Model Van Der Waals Interactions — •Florian Göltl and Jürgen Hafner — Faculty for Physics, University of Vienna, Austria

In this work we investigate the performance of different levels of theory to describe the adsorption of alkanes in chabazite, a mineral from the zeolite family. Modeling this problem is an especially challenging task, since, even though there is a very weak bond between the adsorption site (in our case an H- or Na- atom) and the alkane, the bonding is dominated by van der Waals (vdW) interactions between the alkane and the zeolite wall.

Even though vdW-interactions are not included in standard density functional theory (DFT), several ways to include them in DFT and post-DFT methods were proposed. In this work we compare the performance of (i) DFT in its generalized gradient approximation after Perdew, Burke and Ernzerhof (PBE), (ii) PBE with an added force-field after Grimme (PBE-d), (iii) the van der Waals density functional after Dion et al. (vdW-DF), (iv) the Adiabatic Connection Fluctua-

tion Dissipation Theorem in its Random Phase Approximation (RPA), (v) a modified form of the RPA, where the Hartree Fock exchange-contribution is evaluated selfconsistently (RPA-HF) and (vi) 2nd order Møller Plesset perturbation theory (MP2).

We give a critical discussion of differences in structural parameters, charge distribution and energetics and propose an improved way to compare the theoretically obtained results with experiment.

MM 7.2 Mon 14:45 IFW B

Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional — •Carlos Pinilla[1], Emilio Artacho[2], Jose Soler[3], Tristan Youngs[4], and Jorge Kohanoff[4] — [1]ICTP, Strada Costiera 11, 34151, Trieste, Italy — [2]Dept. Earth Sciences, University of Cambridge, CB2 3EQ, UK — [3]Universidad Autonoma de Madrid, Cantoblanco, Spain — [4]ASC, Queens University Belfast, BT7 1NN, UK

The role of dispersion interactions in imidazolium-based room-temperature ionic liquids is studied within the DFT framework, using a recently developed non-empirical functional[1], as efficiently implemented in SIESTA[2]. We present results for the equilibrium structure and lattice parameters of several crystalline phases, finding a general improvement with respect to LDA and GGA. In particular, equilibrium volumes reproduce experimental values to unprecedented accuracy. Intra-molecular geometries are retained, while intermolecular distances and orientations are improved relative to LDA and GGA. The quality is superior to that from tailor-made empirical VDW corrections. We provide some insight into the issue of polymorphism of [bmim][Cl] crystals, and present results for the geometry and energetics of [bmim][Tf] and [mmim][Cl] clusters. By comparing to quantum chemical MP2 calculations on clusters, we validate VDW geometries and binding energies. Finally, we also analyze the performance of an optimized version of this functional[3]. [1] M. Dion et al. Phys. Rev. Lett. 92(2004).[2] G. Román-Pérez et al. Phys. Rev. Lett. 103(2009).[3]J. Klimes, D. et al. J. Phys.:Cond. Mat. 22(2010)

MM 7.3 Mon 15:00 IFW B

Treatment of strongly correlated systems within the framework of reduced density matrix functional theory — •Sangeeta Sharma, J. K. Dewhurst, and E. K. U. Gross — Max-Planck-Institut für Mikrostrukturphysik, D - 06120 Halle

One of the most dramatic failures of the usual local density approximation or generalized gradient type approximations to the exchange-correlation functional of density functional theory is the incorrect prediction of a metallic ground state for the strongly correlated Mott insulators, of which transition metal oxides (TMOs) may be considered as prototypical.

In the present work we extend reduced density matrix functional theory (RDMFT) to the case of solid-state systems and introduce a new functional for their accurate treatment [1]. Furthermore, a method for calculating the spectrum of extended solids within RDMFT is presented. An application of this method to the strongly correlated TMOs demonstrates that (i) an insulating state is found in the absence of magnetic order and, in addition, (ii) the interplay between the charge transfer and Mott-Hubbard correlation is correctly described. In this respect we find that while NiO has a strong charge transfer character to the electronic gap, with substantial hybridization between t_{2g} and oxygen-p states in the lower Hubbard band, for MnO this is almost entirely absent [2]. References 1. S. Sharma, J. K. Dewhurst, N. N. Lathiotakis and E. K. U. Gross Phys. Rev. B 78, 201103 Rapid Comm. (2008) 2. S. Sharma, S. Shallcross, J. K. Dewhurst and E. K. U. Gross cond-mat/0912.1118

MM 7.4 Mon 15:15 IFW B

Understanding Macroscopic Fiber Systems with Statistical Mechanics Concepts — •Nava Schulmann — Institut Charles Sadron, Strasbourg, France

Many natural systems such as cellulose fibers, hair, DNA, or manufactured materials like ropes or wires are made from fibers. The mechanical and statistical mechanic behavior of individual fibers is now well understood and can be described by the physical concepts of torsion, extension and curvature rigidities, and by the topological concepts of twist and writhe. The properties of matter made by many interacting microscopic fibers have also been investigated to some extent, particularly in the limit where fiber rigidity is small enough for thermal forces to play a predominant role. Macroscopic or more rigid systems, where temperature plays a negligible role are much less understood. We have studied fiber stacks [Europhys. Let., 2003, 64, 647], and shown that statistical physics concepts from the thermal systems can be used to understand many properties of the macroscopic systems. In particular, we have shown that the frozen curvature heterogeneities give rise to an effective temperature that controls material properties such as stack compressibility or assembly shape. The aim of this project is to confront the mean-field theoretical predictions for nearly-aligned fiber stacks with numerical simulations. In particular, we want to understand the accuracy of the effective temperature analogy and the limits of the mean-field approximation.

MM 8: Liquid and Amorphous Metals II

Time: Monday 14:30–15:30 Location: IFW D

MM 8.1 Mon 14:30 IFW D

First measurements of the diffusion coefficient in shear bands — •Joachim Bokeloh, Sergiy Divinskiy, Gerrit Reglitz, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Although the occurrence of shear bands during plastic deformation of metallic glasses was discovered early on and in spite of the extensive research done on the formation of shear bands and their behaviour during plastic deformation, they remain a fairly unknown entity. A key factor in this is the difficulty in accessing the actual physical properties of the shear bands. This is reflected in the very limited number of publications that report experimental data on shear band properties as opposed to the large number of publications that approach shear bands from simulation. In this presentation, experimental data on the diffusion in shear bands has been obtained using the radiotracer method that is conventionally utilized for determining grain boundary diffusion coefficients. Utilizing the tracer method on the post-deformed specimen serves analysing a lower bound of the diffusivity that was present during the shear band formation, i.e. during plastic deformation. Yet, the experimental results indicate unambiguously that even in the post-deformation state the diffusivity is largely enhanced as compared to the volume diffusion in metallic glasses.

MM 8.2 Mon 14:45 IFW D

Thermophysical properties and medium-range order of liquid Ni-Si alloys — Yongjun Lü and •Peter Entel — Faculty of Physics and Center for Nanointegration, CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

The thermophysical properties of liquid Ni-Si alloys as a function of silicon concentration are investigated using molecular dynamics simulations. The temperature dependent enthalpy and density indicate the occurrence of crystallization in Ni-5%Si and Ni-10%Si and glass transitions for 20% and 25%. With the Si concentration increasing from 5 to 25%, the self-diffusivities decrease and viscosities increase with more non-Arrhenius temperature dependences in the low-temperature region, suggesting fragile characteristics of these alloys. Moreover, a shoulder peak emerges between the first and second peak in all radial distribution functions before crystallization or glass transition. Positions of shoulder, second and third peaks relative to the nearest neighbor peak are consistent with a global packing model [1], showing the incompact local translational symmetry. The atomic arrangement prefers a special bond angle distribution and displays orientational order. Therefore, the medium-range order of liquid Ni-Si can be described as a combination of local translational and orientational orders. This local packing structure becomes more compact with addition of more Si atoms, suppressing the formation of crystalline order.

[1] X. J. Liu et al. Phys. Rev. Lett. 105, 155501(2010)

MM 8.3 Mon 15:00 IFW D

The effect of quenching on the mechanical properties of Ti40Zr10Cu34Pd14Sn2 bulk metallic glass — •Na Zheng[1], Mihai Stoica[1], Mariana Calin[1], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 27 01 16, D-01069 Dresden, Germany — [2]TU Dresden, Institute

of Materials Science, D-01062 Dresden, Germany

Ti40Zr10Cu34Pd14Sn2 bulk metallic glass (BMG) exhibits large glass forming ability and good mechanical properties. Upon compression tests, it was found that the plastic strain is 3.5% and the corresponding fracture stress is around 2050 MPa. Annealing at elevated temperatures followed by rapid quenching is an effective way to tailor the microstructure of BMG and then change the mechanical properties. In this work, Ti40Zr10Cu34Pd14Sn2 BMG with the diameter of 2 mm was obtained by suction casting. Differential Scanning Calorimetry (DSC) investigations preformed at 20 K/min heating rate reveal the glass transition temperature (Tg) of 673 K and the first onset temperature of crystallization (Tx1) of 726 K. After annealing at temperatures slightly before Tg and in the supercooled liquid region (Tg-Tx1), the BMG samples were quenched in water. The aim is to study the effect of quenching on the mechanical properties of Ti40Zr10Cu34Pd14Sn2 BMG. Additionally, the fracture morphology of these samples is also investigated.

MM 8.4 Mon 15:15 IFW D

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

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

MM 9: Topical Session TEM III

Time: Monday 15:45–17:30 Location: IFW A

Topical Talk MM 9.1 Mon 15:45 IFW A

Advanced electron microscopy and first-principles calculations: New insights into materials science on the atomic scale — •Rolf Erni — Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

New electron optical devices, such as monochromators, spherical and chromatic aberration correctors, have boosted the resolution in (scanning) transmission electron microscopy. In parallel, the revolutionized optics has increased the sensitivity of the imaging techniques to a level where, for instance, the dynamics of individual atoms can be monitored, employing a microscope setting tailored to the material to minimize radiation damage. This overall progress has opened the possibility to reliably study smaller materials systems; while typically in conventional microscopy millions of atoms constitute a high-resolution micrograph, the new optics allows for monitoring systems that are merely defined by a few hundred atoms, which indeed is a requirement if the functionality of a nano-device needs to be analyzed. As a consequence, nowadays microscopy data can provide direct input for first-principles calculations. Indeed, combining the theoretical and the experimental approach leads to synergies that simplify finding answers for new observations. The advantage of this tandem approach is demonstrated by discussing the dynamics and stability of ad-atoms and ad-molecules on suspended graphene. Moreover, while most atomic-scales studies are confined to two-dimensional projections, an outlook is given on how the third spatial dimension could be explored.

Topical Talk MM 9.2 Mon 16:15 IFW A

Quantitative STEM: Composition mapping in InGaN — •Andreas Rosenauer[1], Thorsten Mehrtens[1], Knut Müller[1], Katharina Gries[1], Marco Schowalter[1], Stephanie Bley[1], Parlapalli Venkata Satyam[1], Christian Tessarek[1], Kathrin Sebald[1], Moritz Seyfried[1], Jürgen Gutowski[1], Adrian Avamescu[2], Karl Engl[2], and Stephan Lutgen[2] — [1]Universität Bremen, Institut für Festkörperphysik, D-28359 Bremen — [2]OSRAM Opto Semiconductors GmbH, D-93055 Regensburg

In this contribution we demonstrate that measurement of In concentration in InGaN layers is possible by scanning transmission electron microscopy Z-contrast imaging as the tendency to form In rich regions due to electron beam irradiation is smaller than for parallel beam illumination. The suggested method is based on comparison of intensity normalized with respect to the incident electron beam with image simulation computed with the STEMsim program. In InGaN, static atomic displacements are caused by the different covalent radii of the metal atoms. These displacements are computed by structure optimization of InGaN supercells using empirical potentials in the Stillinger Weber parameterization. The suggested procedure is validated using an InGaN layer with 7 % homogeneous In concentration by comparison of the STEM results with results obtained by other methods. Despite a high convergence angle of the incident electron beam, simulation of an abrupt interface between InGaN and GaN shows that artificial blurring of the interface is significantly reduced by electron channelling.

MM 9.3 Mon 16:45 IFW A

TEM studies of PbS-ZnS/ZnO quantum confinement structures for solar cells — •Peter G. Schindler[1], Neil P. Dasgupta[2], Orlando Trejo[2], Christian Rentenberger[1], Thomas Waitz[1], Fritz B. Prinz[2], and Hans-Peter Karnthaler[1] — [1]University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria — [2]Stanford University, Dept. of Mechanical Engineering, Stanford, CA 94305, USA

Research to maximize the efficiency of solar cells used for photovoltaic power generation is a timely issue. Si technology uses only a limited range of frequencies of the solar spectrum. To overcome this, quantum confinement solar cells give the opportunity for band gap engineering by quantum effects facilitated by dimensions in the nm range. We report on a transmission electron microscopy (TEM) study of layers of PbS and ZnS/ZnO deposited by atomic layer deposition. To prepare cross-section TEM samples the structures were glued together face to face to protect them. To achieve wedge shaped TEM foils with an extremely shallow angle the samples were mechanically polished and in a last step softly polished with Ar^+ ions. The cross-sectioned multilayer quantum dot (QD) structure, its composition and morphology were investigated with different TEM techniques, e.g. high resolution TEM, and high angle annular dark field. The results are: The size of the QDs is in the range of the thickness of the layers which is about 2-5 nm. The QDs are faceted and either of small round shape or elongated along the layers. The range of size variations of the QDs increases with distance from the substrate resulting in the desired variation of band gaps.

MM 9.4 Mon 17:00 IFW A

Annealing in InGaNAs studied by TEM three-beam imaging — •Knut Müller[1], Marco Schowalter[1], Michael Hetterich[2], Dongzhi Hu[2], Daniel Schaadt[2], Philippe Gilet[3], Kerstin Volz[4], and Andreas Rosenauer[1] — [1]Univ. Bremen, D-28359 Bremen — [2]Karlsruhe Inst. of Techn., D-76131 Karlsruhe — [3]CEA-LETI, F-38054 Grenoble — [4]Univ. Marburg, D-35032 Marburg

A 3-beam TEM image formed by 000, 200, and 220 is used for simultaneous atomic-scale measurement of In and N in an $In_{0.28}Ga_{0.72}N_{0.02}As_{0.98}$ quantum well. In this setup, subsequent diffractogram filtering yields 200 and 220 lattice fringes that are not coupled by nonlinear imaging. Images are acquired with a FIB-fabricated, L-shaped objective aperture in a Cs-corrected Titan

80/300. Indium and nitrogen contents are determined by comparing chemically sensitive 200 fringe amplitude and 220 strain with simulated reference data., which includes bonding and static atomic displacements (SAD). It is demonstrated that bonding improves accuracy up to 30%, and that SAD cause absorption in Bragg beams due to Huang scattering, which is treated by additional absorptive form factors. For the present structure, annealing is shown to cause photoluminescence to increase by a factor of 20 and to blue-shift by 65nm. Using our 3-beam method, this can be assigned to a dissolution of In- and N-rich regions in favour of a homogenisation of layer thickness and -stoichiometry.

MM 9.5 Mon 17:15 IFW A

Quantitative evaluation of Avrami-type crystallization in a thin GeSi film using double wedge geometry — •Florian Niekiel and Erdmann Spiecker — CENEM, Universität Erlangen-Nürnberg, Erlangen, Germany

A key to understanding and controlling thin film growth processes and properties is the knowledge of the variation in structure with distance from the substrate. Transmission electron microscopy (TEM) is known as a powerful tool for characterization of thin films structures. By combining plan-view and cross-section analysis a qualitative view of the three-dimensional (3D) film structure can be obtained. However, neither of the two geometries is compatible with the need for quantitative characterization of the structural, crystallographic or compositional parameters that define the thin film. We have recently developed a new double wedge sample preparation technique that enables plan-view TEM investigation of large areas at each depth in the film. Based on a quantitative evaluation of image series statistically relevant data on the 3D film structure can be obtained. Here, we demonstrate the technique for a GeSi film that first started to grow in the amorphous state, then formed crystalline nuclei that expanded with increasing distance from the substrate finally replacing all amorphous material in the top part of the film. Quantitative evaluation of extensive image series obtained in double wedge geometry allowed us to determine the relative fraction of crystalline material as a function of distance from the substrate.

MM 10: Computational Materials Modelling III

Time: Monday 15:45–17:30 Location: IFW B

MM 10.1 Mon 15:45 IFW B

Atomistic simulations of dislocations in strontium titanate — •Pierre Hirel[1,2], Matous Mrovec[1,2], and Christian Elsässer[1,2] — [1]Institut für Zuverlässigkeit von Bauteilen und Systemen (IZBS), Karlsruher Institut für Technologie, Kaiserstr. 12, 76131 Karlsruhe (Germany) — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg (Germany)

Strontium titanate (STO) is a perovskite oxide whose large dielectric constant makes it an attractive material for modern microelectronic applications. In contrast to the ongoing interest in electrical properties of STO, its mechanical properties came to the attention of the scientific community only in 2000 after a surprising discovery of a ductile-to-brittle-to-ductile transition. It was found that STO can deform plastically at room temperature, but the properties of dislocations mediating the deformation remain up to now a matter of debate.

The present study investigates the properties of dislocations in STO by means of atomistic simulations. The investigations are based on a multi-scale approach that uses both quantum-mechanical first-principles calculations and classical atomistic simulations with a rigid-ion potential. We compute the core structures of both screw and edge dislocations and analyze possible dissociation types and their relation to macroscopic mechanical behavior. The glide of dislocations under applied stress is studied directly by molecular dynamics simulations as well as indirectly using the nudged elastic band method. Our simulation results are compared to high-resolution transmission electron microscopy observations.

MM 10.2 Mon 16:00 IFW B

Elasticity and Screw Dislocations in W-Re and W-Ta Alloys — •Hong Li[1,2], Lorenz Romaner[2], Claudia Ambrosch-Draxl[2], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahn Straße 12, 8700 Leoben, Austria — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

Using a first-principles approach, the elastic properties as well as the core structure of the 1/2<111> screw dislocation in W-Me (Me=Ta, Re) alloys are investigated from the atomistic point of view. For a range of Ta/Re concentrations the lattice parameter, bulk modulus, and elastic constants are calculated and compared with pure W to study the influence of solute atoms on the elastic properties. A periodic quadrupolar arrangement of the dislocation is employed to model the core structures. We show that W and W-Ta alloys at all concentrations exhibit a symmetric core structure. In contrast, W-Re alloys exhibit a gradual transition to asymmetric cores. Furthermore, the critical stress which has to be applied to move the dislocation at 0K (Peierls stress σ_p) is calculated to determine the mobility of dislocations. The reduction of σ_p and a change of slip plane explain the brittle to ductile transition in W upon Re alloying. However, for W-Ta alloys the reduction of σ_p is found only with high Ta concentrations. Finally, we investigate the correlation between the core symmetry and the γ-surfaces for both W-Me cases.

MM 10.3 Mon 16:15 IFW B

DFT study of impurities at grain boundaries in α-Fe — Elwira Wachowicz and •Adam Kiejna — Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

The effects of several metalloid (B), metalloid-like (C, P) and non-metallic impurities (N, O and S) on structure, energetics and mechanical properties of Σ3 (111) and Σ5 (210) grain boundaries (GBs) in ferromagnetic α-Fe have been studied by density functional theory and the projector augmented wave method. Two different concentrations and positions of impurity atoms at the GB were considered. Most of the impurities enhance the relaxation of the interplanar spacing of the pure grains. Interstitial impurities at both GBs increase separation of the grains while substitutional ones in general either do not alter or decrease it. Segregation of impurity atoms at the GBs and their embrittling/strengthening effect is explored and discussed in terms of its chemical and mechanical components. At the Σ5 GB for all impurity atoms considered the positions in the boundary layer are energetically favored independently of interstitial or substitutional site, whereas the enrichment of the Σ3 GB is favored for the impurities of the interstitial sites as well as for a substitutional P and C. In most cases, impurity atoms both in interstitial and substitutional positions at GBs act as embrittlers. The magnetic moments on the impurities are very small and in most cases align antiparallel to the moments on the neighboring Fe atoms.

MM 10.4 Mon 16:30 IFW B

Simulation der Korngrenzenbeweglichkeit in Aluminium mittels Molekulardynamik — •Volker Mohles und Jian Zhou — Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen

Die Beweglichkeit von Korngrenzen und speziell ihre Temperaturabhängigkeit sind von größter technischer Bedeutung für die Rekristallisatioskinetik in industriellen Wärmebehandlungen. Daher gibt es in der Literatur eine Reihe von Molekulardynamik-Simulationen, in denen Korngrenzen durch eine synthetische, kristallorientierungsabhängige Kraft im Bewegung versetzt werden, um so die Mobilitäten der Korngrenzen abzuleiten. Die Ergebnisse bisheriger solcher Simulationen stehen in Hinblick auf die Temperatur- und Winkelabhängigkeit der Mobilitäten jedoch in starkem Widerspruch zu entsprechenden gemessenen Werten. Im vorliegenden Beitrag wird gezeigt, dass diese Widersprüche aus zwei unabhängigen, gravierenden Ungenauigkeiten der bisherigen Simulations- und Auswertungstechnik resultieren. Es werden Verbesserungen der Methodik vorgestellt, mit denen diese Ungenauigkeiten unterbunden werden können. Am Beispiel simulierter und experimenteller Ergebnisse zu reinem Aluminium wird gezeigt, dass Molekulardynamiksimulationen mit korrigierter Methodik verlässliche Mobilitätswerte für Korngrenzen vorhersagen können.

MM 10.5 Mon 16:45 IFW B

Plasticity of Cu and Pd nanoparticles in nanoextrusion — •Antti Tolvanen[1,2] and Karsten Albe[1] — [1]Institute of Ma-

terials Science, Darmstadt University of Technology, Germany — [2]Department of Physics, University of Helsinki, Finland

Recent transmission electron microscopy experiments have shown how nanoparticles can be encapsulated inside carbon onions and electron irradiation induced contraction of these onions can be used to apply pressure of tens of GPa to the encapsulated particle [1]. If an orifice is opened to the carbon onion, this system can be used to study the extrusion of the encapsulated material through this orifice. Therefore studying the extrusion of metallic nanoparticles from such nanocontainers provides information on the plasticity of individual nanograins. In this study, the results of molecular dynamics simulation of the extrusion of Cu and Pd nanoparticles pressurised in spherical force field mimicking the behaviour of contracting carbon onion are presented. We compare the plastic behavior single-crystalline nanoparticles of Cu and Pd with multiply-twinned nanoparticles. The effects of the low and high stacking fault energies of Cu and Pd, correspondingly, and the effect of twins on the dislocation nucleation and propagation is reported for both metals.

[1] L. T. Sun et al, Phys. Rev. Lett. 101, 156101 (2008)

MM 10.6 Mon 17:00 IFW B

DFT calculation on Fe/ZrO_2-Interfaces — •Jürgen Kutzner and Jens Kortus — Technische Universität Bergakademie Freiberg

Interface structures of the Fe/ZrO_2-system are presented. We investigated several possible orientations and configurations by means of density functional theory. Special emphasis was put on mechanical stability, termination of the different interface-structures and magnetic effects. The energetic comparison gives a view on the order of occurrence. As an addition, some experimental data is presented.

MM 10.7 Mon 17:15 IFW B

Studying grain growth in $SrTiO_3$ by diffraction contrast tomography and simulation — •Melanie Syha[1], Wolfgang Rheinheimer[2], Michael Bäurer[2], Erik M. Lauridsen[3], Wolfgang Ludwig[4], and Daniel Weygand[1] — [1]Karlsruher Institut für Technologie, IZBS, — [2]Karlsruher Institut für Technologie, IKM ,Kaiserstr. 12, 76131 Karlsruhe, Germany — [3]Risø National Laboratory for Sustainable Energy, 4000 Roskilde, Denmark — [4]European Synchrotron Radiation Facility, 38043 Grenoble, France

A comparison of the three dimensional (3D) grain structure in $SrTiO_3$ measured by diffraction contrast tomography (DCT) experiments and mesoscale grain growth simulations is presented. The objective of this study is to explain the recently observed growth anomaly in $SrTiO_3$. The simulations allow for a systematical parameter variation, while the DCT experiments yield fundamental insight on structure and crystallography in 3D. In conjunction, these methods give access to the details of the topological quantities in grain structures and form an appropriate tool to study the influence of interface parameter variations on the grain morphology. The applied simulation tool is a 3D vertex dynamics model capable of handling inclination and misorientation dependent interface properties in structures consisting of several thousand grains. Using existing experimental data on orientation dependent interface energies/mobilities, as well as DCT results on structure, grain/pore shape and crystallography as input, the model has been enabled to depict the microstructural evolution of $SrTiO_3$ during annealing. A detailed comparison with 3D annealing experiments is provided.

MM 11: Liquid and Amorphous Metals III

Time: Monday 15:45–17:15 Location: IFW D

MM 11.1 Mon 15:45 IFW D

Stick-Slip Instabilities in a Zr-based Bulk Metallic Glass — •David Klaumünzer, Robert Maass, Peter Thurnheer, and Jörg F Löffler — Laboratory of Metal Physics and Technology, ETH Zurich, Zurich, Switzerland

At temperatures well below the glass transition, plastic deformation of bulk metallic glasses is characterised by a strong degree of flow localisation and the formation of narrow shear bands. The mechanism by which shear bands form and operate remains subject of debate. We can show that serrated flow observed during compression testing of bulk metallic glasses is remarkably similar to other stick-slip systems. While a common property of these systems seems to be their disordered nature, they essentially bridge a wide range of underlying dimensions, from macroscopic to atomic length scales. The dynamics of individual slip events in a Zr-based metallic glass can be captured by time-resolved compression testing. A careful analysis reveals a wide distribution of event duration in agreement with chaotic dynamical behaviour. A correlation between event amplitude and duration can be established. The results are discussed by applying conventional stick-slip theory to the inhomogeneous deformation behaviour of metallic glasses.

MM 11.2 Mon 16:00 IFW D

A fundamental new approach on structure formation — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Whereas the formation of molecules is well understood the formation of crystalline matter is not. Liquid and amorphous systems are somewhere inbetween. The number of atoms is already huge and hence Schrödingers equation is unable to treat them properly. Thermodynamics fails too due to its incompleteness: the lack of momentum and angular momentum, indispensable incredients of any description of structure formation.

Liquid and amorphous systems are by no mean really disordered, instead show well defined structural order. We show for all the liquid elements along the Periodic Table, known to us, that their structural features are formed under the influence of resonances between global subsystems as there are the Fermi gas of the electrons as one, and the forming static structure as the other one. Both mutually adjust and trigger medium-ranging spherical-periodic order (SPO) in the mean around any atom. The fundamental processes causing this feature may once help us to understand better the formation of long-ranging crystalline order, nucleation and growth. We present a new analysis of all the structural data, discuss the resonance interaction based on momentum exchange as the driving effect which causes bonding as well as anti-bonding states between the global subsystems. We discuss the importance of entropy creation when the total system finally occupies the bonding state.

MM 11.3 Mon 16:15 IFW D

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

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

For thin films of amorphous AlPd alloys, deposited at a temperature around 4 K, the resistivity and the thermopower have been measured from 4 K to 345 K, the atomic structure after annealing to room-temperature by TEM. The thermal stability is largest around 30-40 at%Pd and hence supports our assumption of hybridization of Al-3p electrons with the Pd-4d-states. Comparing the position K_{pe} of the first peak in $S(K)$, the structure factor, with $2k_{\mathrm{F}}$, the diameter of the Fermi sphere, we extract another composition around 60 at%Pd, where again there is an electronic stabilizing effect, but now without hybridization.

MM 11.4 Mon 16:30 IFW D

Relaxation kinetics of a AuCuAgSi bulk metallic glass — •Jonas Bünz and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Au-based bulk metallic glasses that were recently discovered belong to the metallic glasses that provide the highest kinetic stability against devitrification. Additionally, and in contrast to earlier types of metallic

glasses with high stability, the glass transition occurs at rather low temperatures around 100°C. This allows the determination of the temperature dependence of the relaxation time directly with microcalorimetry for a Au50Cu25.5Ag7.5Si17 bulk metallic glass with very high accuracy. The availability of both relaxation data for enthalpy and volume and thermodynamic data for this specific system allows comparing different models for the structural relaxation on the basis of experimental data.

MM 11.5 Mon 16:45 IFW D

Einfluss von Silber und Bismut auf die Viskosität des flüssigen Zinns — •Andriy Yakymovych, Yuriy Plevachuk und Vasyl Sklyarchuk — Institut für Metallphysik, Nationale Ivan-Franko-Universität, Lviv, Ukraine

Blei und bleihaltige Legierungen gehören zu den gefährlichsten Chemikalien für Menschen. Ein von Verfahren bleihaltiger Materialer zu vermeiden, ist neue Lotmaterialien zu finden. Die Kräfte, welche die Struktur im festen Zustand, auch im flüssigen Zustand wirksam sind. Diese Arbeit wird die Forschungsergebnisse der Viskosität, wie eine von strukturell sensibler Eigenschaft, bleifreie Lotmaterialien (Systeme Sn-Ag und Sn-Bi-Ag) präsentiert. Die Wichtigkeit der Forschung ist die Auswirkungen von Silber und Bismut auf die Zähigkeit des Zinn zu untersuchen.

Die Viskosität von Sn, SnxAg100-x und (SnxAg100-x)90Bi10 war mit dem Torsionsviskosimeter gemessen. Die Viskositätzunahme durch zweites Element ist beobachtet. Auf andere Seite auf Isotherme ist geringe Absteigeffekt beobachtet, was ist typisch für eutektische Legierungssystemen.

MM 11.6 Mon 17:00 IFW D

Surface Tension and Reactive Wetting in Solder Connections — •Andre 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. In order to quantify this energy, we measured wetting angles of solder drops as well as surface tension of SnPb solders under systematic variation of composition and gaseous flux at different reflow temperatures. For the latter, we used the sessile drop method placing a solder drop on a glas substrate. From the two independent data sets, the important energy of the reactive interface is evaluated based on Young's equation. Remarkably, although both, the tension between the solder and flux and the wetting angle, reveal significant dependence on solder composition. So the adhesion energy reveals distinguished plateaus which are related to different reaction products in contact to the solder. TEM analysis and calculations of phase stabilities show that there is no Cu6Sn5 for high lead concentrations. The experiments confirm a model of reactive wetting by Eustathopoulos[1].

[1]N. Eustathopoulos; Current Opinion in Solid State and Materials Science, 9 (2005) 152-160.

MM 12: Postersitzung I

Time: Monday 17:30–19:00 Location: P5

MM 12.1 Mon 17:30 P5

Molecular dynamics studies on amorphous CuTi nanoparticles — •Susanne Fichtner and S.G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

It is generally well established that physical properties of materials in reduced dimensions deviate from their macroscopic behavior – particularly due to surfaces and dimensionality. For metallic glasses influences on structure, mechanical properties and the glass transition have to be expected.

We employ classical molecular dynamics simulations using embedded atom method (EAM) potentials for the model glass, CuTi, to address the influence of dimensionality and open surfaces on structure. Starting from an amorphous CuTi cell, which is prepared by quenching from liquid, amorphous particles are prepared by cutting out clusters of various sizes, ranging from 1.4nm to 4nm. After relaxation at different temperatures, changes in the pair and angular distributions are followed. Influences of surfaces and dimensionality, as well as the underlying physical origins on the atomic scale are discussed.

This project is financially supported by the DFG - PAK 63.

MM 12.2 Mon 17:30 P5

Nonlinear effects of damping behavior and activation volume of metallic glasses below to above the glass transition temperature — •Moritz Schwabe, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The idea of a potential energy landscape (PEL) from Stillinger and Weber describes relaxation processes in two ways of stimulation: α-relaxations as a changeover to a new metabasin and β-relaxation as changes within the fine structure of the metabasin. External stress can vary these barriers as discussed by W.L. Johnson and K. Samwer. [1,2] With this background we analyzed creep- recovery measurements at constant temperature to investigate the damping behavior of amorphous PdCuSi below Tg. Furthermore we compare the relation of the glass transition temperature and the apparent activation volume for plastic deformation to external stress and temperature of the fragile glass former PdCuSi and the strong ZrAlCu. Then an exponential, multiplicative relationship of stress and temperature dependence can be suggested. [3] [1] P.G. Debenedetti and F.H. Stillinger, Nature, 2001, 410, 259 [2] W.L. Johnson and K. Samwer, Physical Review Letters, 2005, 95, 195501 [3] M. Schwabe, S. Küchemann, H. Wagner, D. Bedorf and K. Samwer, Journal of Non-Crystalline Solids, doi:10.1016/j.physletb.2003.10.071

MM 12.3 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(Cu_{60}Co_{40})_{1-x}Zr_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D. H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

The binary Cu-Co system exhibits a metastable liquid-liquid miscibility gap and therefore the ternary Cu-Co-Zr system is a promising candidate to form phase separated glass-glass composites. In this work $(Cu_{60}Co_{40})_{1-x}Zr_x$ metallic glasses with $x = 37$ and $x = 32$ were investigated by in-situ small-angle and wide-angle x-ray scattering (SAXS/WAXS) and differential scanning calorimetry (DSC). Certain heat treated samples were additionally investigated by high-resolution transmission electron microscopy (HRTEM). Even for $x = 32$ there are no indications for any kind of phase separation in the as-quenched state within experimental resolution, i.e. the critical temperature T_c for liquid-liquid phase separation has already decreased from 1556 K for binary $Cu_{60}Co_{40}$ to a temperature below the glass transition temperature $T_g = 762(5)K$ found for $(Cu_{60}Co_{40})_{68}Zr_{32}$. Combined in-situ SAXS/WAXS and HRTEM investigations reveal that thermal annealing induces the formation of a composite consisting of nano crystallites embedded in an amorphous matrix.

nano

MM 12.4 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(Cu_{60}Co_{40})_{1-x}Zr_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D. H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

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MM 12.5 Mon 17:30 P5

Combined in-situ SAXS/WAXS and HRTEM Study on Crystallization of $(Cu_{60}Co_{40})_{1-x}Zr_x$ Metallic Glasses — •B. Schwarz[1], U. Vainio[2], N. Mattern[1], S.W. Sohn[3], D.H. Kim[3], and J. Eckert[1] — [1]Leibniz-Institute IFW Dresden, Institute for Complex Materials — [2]HASYLAB at DESY, Hamburg — [3]Department of Metallurgical Engineering, Center for Noncrystalline Materials, Yonsei University, Seoul, South Korea

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MM 12.6 Mon 17:30 P5

Investigation of the viscosity for Bi-Sn(Zn) liquid alloys — •Andriy Yakymovych, Oleg Volkov, and Petro Yakibchuk — Department of Metal Physics, Ivan Franko National University of Lviv, Lviv, Ukraine

In the present study we have determined the viscosity with use of expressions for a polydisperse hard-sphere fluid (theory) and the high-temperature viscometer (experiment). According to the used theory, we present atoms in binary metallic alloy as a mixture of two subsystems of polydisperse hard spheres which interacts each other via contact potential only. Such assumptions lead us to the fact that we can express viscosity of this system using analytical equations and integrals they contains can be presented by simple mathematic functions for well-defined size distributions of polydisperse particles or by simple numeric scheme in general. Studding different cases of size-distribution in one-component systems we found that viscosity limit (value of average hard sphere volume fraction when viscosity turns to infinity) slightly moves down to zero.

In this work we provide calculations for binary alloys and try to analyze our results by comparison them with real alloys. The experimental measurements were carried out by a torsional oscillation viscometer. The viscosity of Bi-Sn liquid alloys has been studied in the vicinity of eutectic concentration and in vicinity of the demixing curve for Bi-Zn system, respectively.

MM 12.7 Mon 17:30 P5

Vitreous tantalum oxide films on glassy tantalum thin film — •Michael Scheele, Kevin Stella, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Thin amorphous tantalum films are prepared on Si(111) substrates in a metallic glassy state. The amorphous monoatomic state of the film is characterized by X-ray diffraction studies. The glassy state leads to a negative **t**emperature **c**oefficient of the **r**esistivity (TCR) for low sample temperatures $< 200\,K$ which is attributed to incipient localization. Above 200 K a positive TCR is observed as expected for a normal Boltzmann transport regime. The glassy metal tantalum can be oxidized by an electrochemical method, forming a vitreous highly temperature stable tantalum oxide. These oxides can be used as an internal barrier in thin film electronic devices.

MM 12.8 Mon 17:30 P5

Interfacial tension and wetting at the liquid-liquid interface in Al-Bi, Al-In and Al-Pb monotectic alloys — •Ivan Kaban[1], Markus Köhler[2], Lorenz Ratke[2], Walter Hoyer[3], Norbert Mattern[1], and Jürgen Eckert[1] — [1]IFW Dresden, Institute for Complex Materials, P.O.B. 270116, D-01171 Dresden, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), D-51170 Köln, Germany — [3]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany

Aluminium alloys with Bi, In or Pb are characterized by a large miscibility gap in the liquid state. They solidify at normal conditions into layered structures, which is the main shortcoming in a view of practical applications. A crucial role in the demixing process is played by the wetting, liquid-liquid interfacial energy and density difference of the coexistent liquid phases. In this contribution we present the results of the experimental investigations of the density, interfacial tension, and wetting of Al2O3, ZrO2 and TiB2 ceramics at the liquid-liquid interface in Al-Bi, Al-In and Al-Pb alloys. The wetting experiments suggest that Al2O3, ZrO2 and TiB2 particles could be used for the nucleation of a minority phase in the Al-In and Al-Pb immiscible alloys.

MM 12.9 Mon 17:30 P5

Investigation of Real Space Orbital Free Density Functional Theory for the Study of Large Systems — •Jade Mackay, Rainer Backofen, and Axel Voigt — Institute for Scientific Computing, Dresden, Deutschland

A frequently encountered issue in computational materials science is the balance of calculation size and accuracy. The accuracy of the popular Kohn-Sham DFT methods is very impressive. However, interest in systems consisting of tens of thousands, or millions of atoms is growing. Alongside the drive for larger systems, attention is being paid to the consideration of real space formulations. Such formulations have value not only in terms of performance for the study of non-periodic systems (surfaces, clusters, defects), but also when integration with macroscopic modelling is being considered. The Orbital Free DFT (OFDFT) approach of Thomas and Fermi has significant potential for the study of large systems, and readily facilitates a real space implementation. In this we work present results obtained from our implementation of a real space OFDFT formulation using the AMDiS parallel finite elements toolkit.

MM 12.10 Mon 17:30 P5

Generation of polarizable force fields for molecular dynamics simulations of metal oxide systems with long-range interactions — •Philipp Beck, Peter Brommer, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The simulation of oxide systems is computationally much more demanding than that of metals or covalent materials due to long-range electrostatic interactions. We use the Wolf [1] direct, pairwise r^{-1} summation method with spherical truncation for Coulomb interactions and in addition extend it to dipolar interactions. The polarizable oxygen atoms are described with the Tangney-Scandalo [2] (TS) interaction force field where the dipole moments are determined by iteration to a self-consistent solution. After first simulation results [3] for microstructural and thermodynamic properties of silica with the original TS force field, we now present a method to develop polarizable force fields which reparametrize the potentials of the TS approach. The method can be applied to arbitrary metal oxides. Our results agree with experiment and former simulation issues, but reduce the simulation time dramatically due to the linear scaling properties of the Wolf summation.

[1] D. Wolf *et al.*, J. Chem. Phys. **110**, 8254 (1999).
[2] P. Tangney and S. Scandalo, J. Chem. Phys. **117**, 8898 (2002).
[3] P. Brommer, P. Beck, A. Chatzopoulos, F. Gähler, J. Roth and H.-R. Trebin, J. Chem. Phys. **132**, 194109 (2010).

MM 12.11 Mon 17:30 P5

Frozen phonon calculations confirm electron-phonon coupling in $Fe_{1-x}Co_xSi$ — •Wilfried Wunderlich[1] and Dirk Menzel[2] — [1]Tokai University, Fac. Eng., Material Science Department, Kitakaname 4-1-1, 259-1292 Hiratsuka, Japan — [2]TU Braunschweig, Inst. f. Physik d. Kondensierten Materie, Mendelssohnstr. 3, 38106 Braunschweig, Germany

Thermoelectric measurements of the Seebeck voltage were performed

on $Fe_{1-x}Co_xSi$ single crystals under large temperature gradient [1]. They show an increase of a positive Seebeck coefficient as a function of Co-concentration for $x < 0.05$ up to 0.2 mV/K and a decrease for $0.05 < x < 0.2$, and again an increase until $x < 0.5$ and a decrease for $x > 0.7$. The first increase is related to the semiconductor-metal transition, while the second increase around $x = 0.6$ corresponds to a paramagnetic ordering state and is discussed as caused by magnon-phonon-coupling. For each phonon mode several **q**-vector variants were generated, and using these frozen phonons DFT-GGA calculations using VASP were performed. The difference in bond-length spectrum in the presence of phonons changed the electronic bandstructure remarkably. Instead of the 200 meV wide band-gap in the case without phonons, flattening of the electronic bands and broadening of the DOS is observed. From these investigations the electron-phonon coupling constant can be derived.

[1] W. Wunderlich et al., Mater. Res. Soc. Symp. Proc. (2009) Vol. 1128-U01-10 pp. 1-6.

MM 12.12 Mon 17:30 P5

***Ab initio* calculation of variable saddle point energies for atom jumps in $L1_2$ ordered Ni_3Al** — •Martin Leitner[1,2], Doris Vogtenhuber[3], Raimund Podloucky[1], Wolfgang Pfeiler[2], and Wolfgang Püschl[2] — [1]University of Vienna, Faculty of Chemistry, Department of Physical Chemistry — [2]University of Vienna, Faculty of Physics, Department Dynamics of Condensed Systems — [3]University of Vienna, Faculty of Physics, Department of Computational Materials Science

Kinetic Monte-Carlo simulation (KMC) in alloys is as good as the jump frequencies provided. According to transition state theory they are determined by a Boltzmann factor with the energy barrier to be surmounted, which is the difference between a saddle point and the initial state. This energy barrier explicitly depends on the atomic neighborhood of both states, especially on the configuration of the saddle point state. As an example for our arguments we take $L1_2$-ordered Ni_3Al. It represents a class of technologically interesting intermetallic compounds where the highly ordered state leads to favorable properties (high-temperature strength, corrosion resistance,...). As in all fcc-type structures, atoms which jump into a nearest neighbor vacancy have to pass a four-atom window of common nearest neighbors. We discuss the substantial influence of the occupancy of this window on jump probabilities. For a classification of jump types, energy profiles were calculated from *ab initio* by using the VASP code. These results were entered into example KMC-simulations, demonstrating the large impact of variable saddle point energies on overall and detailed kinetics.

MM 12.13 Mon 17:30 P5

FeN_4 defects in carbon nanostructures: a comparative study with Fe-porphyrin and Fe-phthalocyanine molecules. — •Ingrid Ibagon[1] and Hélio Chacham[2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Deutschland — [2]Universidade Federal de Minas Gerais, Belo Horozinte, Brazil

In this work we conducted a comparitive study between the Fe-porphyrin and Fe-phthalocyanine molecules and carbon nanostructures with FeN_4 defects using first principles calculations based on the Density Functional Theory. For all systems, we performed calculations varying the total charge. In the case of Fe-porphyrin and Fe-phthalocyanines we studied the neutral systems and those resulting from the addition or remotion of one electron and, in the case of the carbon nanostructures we added a quantity of charge per carbon atom equivalent to each case studied for the molecules. We observed a tendency of the iron atom to maintain its charge constant when the total charge of the system changes, while the spin magnetic moment of the system changes with the total charge. The systems have spin magnetic moment equal to $2\mu_B$ when they are neutral, but it increases (decreases) when electrons are removed (added) from (to) the system.

MM 12.14 Mon 17:30 P5

Preliminary theoretical results on the solubility of ZnO — •Svea Sauer, Susan Köppen, Lucio Colombi Ciacchi, Christof Köhler, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany

The toxicity of zinc oxide nanoparticles towards macrophage and epithelial cells is directly linked to their solubility in the surrounding solute. In this context a higher solubility was found for nanoparticles dissolved in cell culture media compared to nanoparticles in pure water [1]. Therefore it is crucial to understand the interactions at the solid-water interface that lead to the particle dissolution. Our work puts a focus on the adsorption of different ions on the (10-10) zinc oxide surface in an aqueous environment. The employed ions range from simple anions to more complex molecules like dihydrogen phosphate. Ab-initio Molecular Dynamics simulations using a (4x2) slab model with a pre-adsorbed water layer are carried out in order to investigate the adsorption geometries. To simulate the dissolution of single Zn-atoms from the surface in the presence of different adsorbates a Metadynamics approach as implemented in CPMD is chosen. As the starting point we chose the dissolution of a single Zn-atom from the surface in the absence of adsorbed ions. Preliminary results are shown.

[1]T. Xia et al. ACS Nano 2(10), 2121 (2008)

MM 12.15 Mon 17:30 P5

Structures of metal electrodes at the solid-liquid interface studied by density functional theory — •Xiaohang Lin — Institut für Theoretische Chemie of Universität Ulm, Ulm

Recently, the operation of an electrochemical atomic-scale quantum conductance switch has been demonstrated, which is controlled by an external electrochemical voltage applied to an independent third gate electrode [1]. However, the microscopic processes underlying this atomic switch are still unclear. Using density functional theory (DFT) calculations, we have addressed the structure of Ag and Pb metal surfaces which are both used as electrode materials for the switch. We have considered the presence of water layers and the self-diffusion on flat and stepped metal surfaces in order to contribute to the understanding of electrodeposition. We find that the substantial difference in the lattice constants between Ag and Pb leads to significant changes, as far as the stable water structure at the metal-water interface is concerned. With respect to the metal diffusion, the DFT results indicate that exchange processes can have considerably lower barriers than hopping processes.

MM 12.16 Mon 17:30 P5

A variable charge transfer model for the molecular dynamics code IMD — •Andreas Chatzopoulos and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

For the efficient simulation of solids which contain electric charges and dipole moments and where, hence, the atoms interact by long-range forces, suitable algorithms must be developed. Examples are oxides or metal-oxide interfaces. For this purpose, our molecular dynamics code IMD[1] was enlarged by a dynamic charge transfer model according to Streitz and Mintmire (SM)[2].
In the model of SM the electrostatic energy contains the charges in second order. The charges are determined by minimization of this energy, taking the constraint of charge neutrality into account. In contrast to SM we solve the minimization by the conjugate gradient method. The long-range interactions are handled by the Wolf summation method[3].

[1] J. Stadler et al. *Int. J. Mod. Phys. C* 8, 1131, 1995.
[2] F. H. Streitz and J. W. Mintmire *Phys. Rev. B*, 50(16): 11996-12003, 1994.
[3] D. Wolf et al. *J. Chem. Phys.*, 110(17): 8254-8282, 1999.

MM 12.17 Mon 17:30 P5

Modellierung digitaler Kornmikrostrukturen — •Stefan Schäfer und Dana Zöllner — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Eine Methode zur Generierung digitaler Kornmikrostrukturen polykristalliner Materialen wird vorgestellt. Basierend auf dem Problem der Kreispackungen in zwei Dimensionen wurde ein Algorithmus entwickelt, der eine dichte Kreislagerung generiert, die einer vorgegebenen Größenverteilung folgt. Die daraus entwickelten Mikrostrukturen auf Kornebene wurden bezüglich der Homogenität metrischer und geometrischer Parameter untersucht. Der Generierungsalgorithmus ist dabei so gestaltet worden, dass einer Erweiterung auf drei Dimensionen problemlos möglich ist.

Anschließend wurden ausgewählte Korngefüge, die jeweils einer anderen Verteilungsfunktion folgen, Kornwachstum mithilfe der Monte Carlo Potts Modell Simulation unterworfen. Besonderes Augenmerk lag dabei auf dem frühen Zeitraum des Wachstums, der dem quasistationären Zustand normalen Kornwachstums vorangeht. Es wurde festgestellt, dass durch geeignete Parameterwahl Mikrostrukturen so erzeugt werden können, dass sie dem späten selbstähnlichen Wachstumsregime der Simulation entsprechen.

MM 12.18 Mon 17:30 P5

Cluster Expansion study of $Fe_xNi_yAl_{1-x-y}$ alloys — •Georg Kastlunger, David Reith, Markus Stöhr, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

Cluster expansion (CE) is the state of the art tool to derive concentration dependent properties of alloys with the precision of density functional theory calculations. In this work we apply CE for a ternary system to study thermodynamical phase stabilities for $Fe_xNi_yAl_{1-x-y}$ alloys crystallizing in bcc-based structures. For studying Ni-Al precipitations in Fe (steel) the concentration range was defined correspondingly. On the basis of DFT total energy calculations for about 350 compounds we derived the effective cluster interaction energies (ECI) by a genetic algorithm employing the UNCLE (UNiversal CLuster Expansion) code[1]. After an extensive ground state search the stable phases and their convex free energy hull were identified. For constructing the phase diagram at finite temperatures the converged ECIs were used in both, canonical and grand-canonical Monte-Carlo simulations.

[1] D. Lerch, O. Wieckhorst, G.L.W. Hart, R.W. Forcade, and S. Müller, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009).

MM 12.19 Mon 17:30 P5

Molecular dynamics simulations of tensile tests in Al_2O_3 with new polarizable force field — •Stephen Hocker[1], Philipp Beck[2], Siegfried Schmauder[1], and Hans-Rainer Trebin[2] — [1]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre, Universität Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

We apply the force matching method to generate a potential for molecular dynamics simulations of Al_2O_3. The Wolf summation method is used for Coulomb interactions. In contrary to previous potentials the polarizability of oxygen atoms is taken into account by iteration to a self-consistent solution of the dipole moments. The potential is optimized to reproduce the forces in relaxed and strained Al_2O_3 configurations. We apply the developed potential to simulate tensile tests of Al_2O_3 with (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ tension axes. Stress strain curves are compared with ab initio results and previous molecular dynamics simulation results of Al_2O_3.

MM 12.20 Mon 17:30 P5

Phonon Contribution to the Thermodynamics of Pure and Mixed Clusters in bcc-Fe — •Mina Talati[1], Matthias Posselt[1], Giovanni Bonny[2], Ahmed Tamer Al-Motasem[1], and Frank Bergner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O.Box 510119, D-01314 Dresden, Germany — [2]Nuclear Materials Science Institute, SCK-CEN, Boeretang 200, B-2400 Mol, Belgium

The irradiation-enhanced nanostructural evolution in reactor pressure vessel steels is a multiscale phenomenon. It can be effectively studied by rate theory for which necessary parameters must be obtained through atomistic simulations. The present work focuses on the phonon contribution to the thermodynamics of nanoclusters consisting of vacancy and/or Cu. In all calculations the most recent Fe-Cu interatomic potential developed by Pasianot and Malerba is employed. The vibrational density of states determined by the dynamical matrix method is used to calculate the phonon contribution to free energy of formation and free binding energy of the clusters. Pure bcc-Fe and pure fcc-Cu are used as references in the calculation of the free energy of formation. The vibrational contribution to the total free energy of these metals determined in this work is compared with available CALPHAD data and with literature data obtained by first-principle methods or interatomic potentials. In the case of pure vacancy clusters and for many mixed vacancy-Cu clusters the absolute value of the total free binding energy decreases with increasing temperature. Pure Cu clusters show the opposite behavior.

MM 12.21 Mon 17:30 P5

Electronic Structure of the Doped fcc- C60 Compound of Solid fcc-C60: Ab Initio Calculations — •Samaneh Javanbakht[1] and Saied Jalali Asadabadi[2] — [1]Department of Physics, Faculty of Science, University of Isfahan (UI), Isfahan 81744, Iran — [2]Department of Physics, Faculty of Science, University of Isfahan (UI), Isfahan 81744, Iran

Electronic and structural properties were calculated for the fcc-C60 compound. The calculations were performed within the density functional theory (DFT) employing the augmented plane waves plus local orbital (APW+lo) method as implemented in the WIEN2k code. The C60 clusters were then positioned on the lattice sites of the fcc taking into account the highest symmetry. The carbon atoms were fully relaxed to minimize the interatomic forces. Single and double bond lengths were then calculated using the relaxed atomic positions. Total density of states (DOS) was calculated. We also doped an additional carbon atom as an impurity into the C60 clusters. Recalculating the bonds of this doped structure, we observed that the distinction between double and single bonds becomes less important as charge transfer proceeds in the fcc crystal. Moreover; we have calculated the bang gap of fcc-C@C60,and we realized that it is reduced incredibly.

MM 12.22 Mon 17:30 P5

Extending the Cluster Expansion by vibrational free energies — •David Reith, Markus Stöhr, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

The Cluster Expansion technique allows to carry over the precision of density functional theory (DFT) calculations to systems consisting of 10^6 - 10^9 atoms [1]. It is based on DFT total energies of properly chosen input structures with a common basic lattice. The effective cluster interaction energies (ECI) are derived from CE fitting criteria and then enter into Monte Carlo (MC) simulations for e.g. deriving phase boundaries. By adding vibrational free energies to DFT total energies the ECIs become temperature dependent which strongly influences the CE+MC treatment. The temperature dependent extension of CE is demonstrated on the binary $Fe_{1-x}C_x$ alloy system, for which it turns out that including the vibrational free entropy strongly increases the solubility of Cu in Fe-rich (steel) alloys. We discuss the complications and strategies which have to be followed for deriving the ECIs and for combining CE with temperature dependent ECIs and MC. For the CE+MC calculations we used the UNCLE code [1] and a direct force constant approach for deriving the phonon spectra [2] for each of the DFT input structures.

[1] D. Lerch, O. Wieckhorst, G.L.W. Hart, R.W. Forcade, and S. Müller, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009).

[2] D. Reith, program package fPHON based on PHON by D. Alfè, 1998.

MM 12.23 Mon 17:30 P5

Molecular dynamics simulations of femtosecond laser ablation in copper — •Carolina Trichet Paredes, Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

Femtosecond laser ablation of copper is investigated by using a hybrid simulation scheme. Two equations are solved simultaneously: One for the electronic system, which accounts for laser energy absorption and heat conduction, the other for the dynamics of the lattice where the ablation process takes place. For the electron-temperature a generalized heat-conduction equation is solved by applying a finite difference scheme. For the lattice properties, e.g. pressure, density or temperature, we use common molecular dynamics. Energy transfer between the subsystems is allowed by introducing an electron-phonon coupling term.

Spallation instead of ablation as a ruling phenomenon for thin copper films of various thicknesses was observed. However, it will be shown that the heat conduction plays a crucial role: By changing its value a transition from spallation to ablation occurs. Besides, the ablation rates and cluster size distribution of the ablated material will be compared to recent experiments.

MM 12.24 Mon 17:30 P5

Heat capacity of aluminum nitride phases from *ab initio* calculations — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The ability to calculate thermodynamical material properties on *ab initio* level is an important preliminary for the accurate prediction of phase diagrams.

We present results on the heat capacity of the wurtzite and rocksalt phases of aluminum nitride. The isochoric heat capacity C_V is obtained from harmonic phonon calculations using density functional perturbation theory. In the quasi-harmonic approximation, the isobaric heat capacity C_p is then obtained from C_V via the thermal expansion coefficient. The latter is calculated (i) directly from the mode Grüneisen parameters using phonon calculations at several volumes and (ii) estimated from molecular dynamics.

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Kristallen bei extrem hohen Drücken und Temperaturen

MM 12.25 Mon 17:30 P5

Density functional theory study of LO-TO splitting of vibrational modes of insulating compounds — •Marcel Hieckel, David Reith, and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

We present results of density functional theory (DFT) calculations for vibrational properties of insulating compounds derived by the force constant method [1]. For the exchange-correlation functional the generalized gradient approximation as well as a hybrid functional were used. The LO-TO splitting in ionic solids is due to the long range Coulomb interactions which is caused by the coupling of atomic displacements to the thus generated electrostatic field [2]. The modelling is based on an additional nonanalytic term to the dynamical matrix which depends on the Born effective charges and the dielectric constant whose tensors are derived from DFT calculations of the macroscopic electronic polarization [3]. The results for nonmagnetic ionic compounds are as well as for the transition metal oxides MnO and NiO are presented and compared to experiment. [1] D. Reith, program package fPHON based on PHON by D. Alfè, 1998. [2] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford University Press, 1954. [3] R.W. Nunes and X. Gonze, Xavier, Phys. Rev. B **63**, 155107 (2001).

MM 12.26 Mon 17:30 P5

Comparative analysis of hydrogen-vacancy interactions in Mg and Al based on density functional theory — •Lars Ismer[1], Min Sik Park[2], Anderson Janotti[1], and Chris G Van de Walle[1] — [1]University of California at Santa Barbara, CA 93106 — [2]Missouri University of Science and Technology, Rolla, MO 65409

For hydrogen storage in metals the presence of vacancies in the bulk of the metal and their interactions with atomic hydrogen (H) plays an important role. Using density functional theory we have studied the H-vacancy interactions in hcp-Mg and fcc-Al, two prototypic systems for H storage. We show that a single vacancy can host up to 9 H atoms in Mg and 10 in Al. In going beyond previous theoretical studies we evaluate the concentration of the H-vacancy complexes for different H loading conditions, ranging from low pressures to high pressures of H2 gas. We find strong differences between Mg and Al. In the case of Al, up to 15 % of H atoms are trapped in single vacancies even for very low H pressures, which slows down the diffusion of H atoms. In the case of Mg, these trapping effects are negligible for low H pressures. However, vacancies containing multiple H atoms and H-induced superabundant vacancy formation are predicted to occur in Mg at much lower H loading pressures (about 1 GPa) than in Al (about 10 GPa).

MM 12.27 Mon 17:30 P5

LAMMPS$_{\mathrm{CUDA}}$ - A general purpose MD code — •Christian Trott and Lars Winterfeld — Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany.

Molecular dynamics (MD) simulations are one of the most common computational methods to explore the structure and dynamics of condensed matter systems. They form the basis for investigating many types of materials, ranging from simple atomic liquids, over metal systems to bio-molecules. The advent of easily programmable graphic card processors (GPUs) allows for the development of new codes, which increased the potential workstation performance by more than an order of magnitude. Most of the codes though, are of limited capabilities compared to the well established MD packages like LAMMPS and NAMD. We present our own code, LAMMPS$_{\mathrm{CUDA}}$ (`www.tu-ilmenau.de/lammpscuda`), which aims at providing GPU support for the full LAMMPS functionality. Besides useability and scope of features the main focus of LAMMPS$_{\mathrm{CUDA}}$ is to provide good scaling behavior on GPU based supercomputers such as the Japanese 7168 GPU Supercomputer Tsubame 2.0 (rank 4 in the 2011 TOP500 list of supercomputers). As a result of our development efforts, LAMMPS$_{\mathrm{CUDA}}$ allows for the effective parallel usage of hundreds of GPUs for a single simulation. We present details of the implementation, benchmarks for various material classes such as inorganic glasses, metals and bio-molecules and an investigation of the scaling behavior of LAMMPS$_{\mathrm{CUDA}}$ with varying system size and number of GPUs.

MM 12.28 Mon 17:30 P5

Construction of High-Dimensional Neural Network Potentials Based on Atomic Pairs — •Jovan Jose Kochumannil Varghese and Jörg Behler — Ruhr-Universität Bochum, D-44780 Bochum

An accurate description of the interatomic potential is the crucial step in theoretical simulations. Consequently, a large number of potentials of varying form and complexity has been reported in the literature. Still, for some systems the accuracy that can be achieved is not satisfying. Artificial Neural Networks (NN) have become a promising new tool for the construction of efficient and accurate potentials due to their flexible functional form. We present a new high-dimensional NN approach based on an expansion of the total energy in terms of environment-dependent atom pairs. The advantages and drawbacks of this approach are discussed and compared to the alternative approach employing a summation of atomic energy contributions.

MM 12.29 Mon 17:30 P5

The solubility of carbon in bcc iron under volumetric strain: comparison of DFT and empirical methods — Elisaveta Hristova, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, Germany

With the aim of investigating the interaction of C with dislocations in Fe by large scale molecular dynamics, we evaluate the transferability of different semi-empirical potentials. As a test case the carbon solubility in bcc Fe as a function of lattice strain is studied by ab-initio calculations based on density-functional theory (DFT) and by four different empirical potentials of the embedded-atom method as (EAM) well as the modified EAM (MEAM). Both DFT and (all but one) empirical potential calculations predict that the carbon solubility increases with increasing volumetric strain, up to the maximum applied strain of five percent. However, the enthalpy of formation for this interstitital defect remains positive throughout the whole range of strains. Interestingly, the enthalpy of formation obtained by DFT is much more strain-sensitive than the one obtained by the empirical potentials. The different description of the carbon solubility in the presence of strain fields by the four empirical potentials is due to different parametrization, construction and fitting of the EAM potentials, and in the case of the MEAM to the different formalism including angular dependent bonding.

MM 12.30 Mon 17:30 P5

Efficient ab-initio characterisation of the parameter space of grain boundaries — Naveed Ahmed, Xueyong Pang, Christian Kellermann, •Rebecca Janisch, Holger Dette, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, Germany

A grain boundary is characterised by at least five macroscopic and three microscopic degrees of freedom, the orientation of the grain boundary plane, the misorientation axis and the misorientation angle, as well as the interface translation state. At the same time, continuum modeling of polycrystals requires knowledge of the elastic and plastic properties of all kind of interfaces in their microstructure. To capture the physics of grain boundary sliding, migration and decohesion, these processes should be investigated by atomistic calculations. Especially if the influence of segregated impurities, which can alter the bond character, shall also be described, a quantum mechanical treatment is necessary. However, sampling the above mentioned parameter space ab initio remains a formidable task, even with today's computers. In this paper we will introduce our investigation of the mechanical properties of grain boundaries in aluminum, which aims at replacing such a comprehensive sampling by as few representative calculations as possible. For this we are evaluating a "design of experiment scheme" combined with insight on the role of crystallography that we gain from our ab-initio calculations: On the one hand we are investigating discriminating features in the elastic and plastic response of tilt and twist grain boundaries. On the other hand we are looking for common behaviour that enables a unified treatment and a separation of variables.

MM 12.31 Mon 17:30 P5

Molecular Dynamics Simulations on Carbon Nanoclusters — •Andrew Aird and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

Bulk- as well as nanodiamonds containing impurities are promising candidates for a broad range of applications (quantum computing, magnetometry). A positioning accuracy on the nanometer scale and very small, nanometer sized diamonds containing stable defects are prerequisites. Nowadays, molecular dynamics (MD-) simulations allow the atomistic description of devices with system sizes in the range of 10-100 nm. Using MD simulations together with potentials to describe covalent materials, carbon clusters with and without defects are inves-

tigated. The effect of external mechanical as well as kinetic stress on the structure and stability of the nanodiamonds are of special interest. In addition, low energy implantation processes of nitrogen into bulk- as well as nanodiamonds are explored. The main goal is to optimize these processes with respect to requested target structures.

MM 12.32 Mon 17:30 P5

Quantitative study of the effect of local ordering on the growth kinetics of metallic alloys — M. Guerdane[1], B. Nestler[1], and •H. Teichler[2] — [1]Institute of Reliability of Components and Systems, Karlsruhe Institute of Technology (KIT) — [2]Institute for Materials Physics, University of Göttingen

We illustrate how local ordering in a metallic melt (NiZr) can transform into a massive in-plane ordering at the surface of a crystal (bcc Zr) when commensurablity is given between the solute-centered clusters of the melt and the periodic potential of the crystal surface for a given orientation. Combined molecular dynamics and phase-field simulations allow to estimate quantitatively the influence of the surface effect on the growth kinetics. This study provides a more complete understanding of the relation between the undercooling ability (e.g. in the case of glass forming alloys) and the pronounced local ordering in the melt.

MM 12.33 Mon 17:30 P5

A study of ice crystal growth based on diffuse interface modeling using extended anisotropy formulations — •Marcel Huber, Frank Wendler, and Britta Nestler — Institute of Materials and Processes, Karlsruhe University of Applied Science, Moltkestr. 30, 76133 Karlsruhe, Germany

Though a phenomenon of daily experience, the precise description of ice crystal growth is still lacking. Progress in technical application like ice slurry for cooling, cryodesiccation and freeze casting process in the synthesis of porous ceramics motivate further research. In this work we study equilibrium and off-equilibrium growth of ice crystals in pure water. The solid interfaces evolve due to an interplay of a driving force (pressure change or undercooling) and interface anisotropies with a normal velocity depending on chemical potential, kinetic coefficient and surface stiffness. To define the location of each ice-crystal (of different orientation) and the phase in the computational domain, we introduce non-conserved order parameters, so that the equation for the velocity can implicitly be solved by using a phase-field model of Allen-Cahn type. We pay special attention to the definition of an adequate anisotropy formulation for interface energies and kinetics. We present numerical studies of various formulations including expansions with respect to cubic harmonics and compare the resulting growth shapes under equilibrium conditions to experimental observation. Using these findings, simulations of strongly undercooled dendritic growth of ice are carried out, where the thermal field is also solved in the domain to account for the transport of latent heat.

MM 12.34 Mon 17:30 P5

Phocphate Crystallisation — •Paul Schneider, Andreas Erbe, and Frank Renner — Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland

Chemical reactions forming surface coatings are an important way to protect metals against environmental attack. Besides the relevance for applications, there is a considerable fundamental interest in the nucleation of crystals on surfaces in complex environments. As modern steels contain silicon and aluminium as elements forming passive layers, phosphate crystal growth under acidic conditions on surfaces of aluminium, silicon, and steels containing silicon and aluminium has been investigated. Different fluoride treatments were employed. On Silicon(100) with native oxide layer, a strong etching of pits was observed, with only few phosphate crystals formed on the surface. Results on a steel with aluminium/silicon coating also show a strong etching, and deposition of fluorides on the surface. Differences between pure aluminium and silicon on the one and surfaces in which aluminium and silicon coexists are attributed to the coexistence of metallic and semiconducting crystalline structures in the initial surface. Such coexistence leads to a substantial modification of the pickling attack.

MM 12.35 Mon 17:30 P5

Impact of Ni on degradation of 8.5 mol% Y_2O_3-doped ZrO_2 (8YDZ) — •Benjamin Butz[1], Andreas Lefarth[2], Heike Störmer[2], Annika Utz[3], and Dagmar Gerthsen[2] — [1]CENEM, Universität Erlangen-Nürnberg — [2]Laboratorium für Elektronenmikroskopie, Karlsruhe Institut für Technology (KIT) — [3]Institut für Werkstoffe der Elektrotechnik, KIT

The efficiency of solid oxide fuel cells is influenced by the electrochemical performance of the anode (8YDZ/Ni composite). One criterion is the ionic conductivity of the 8YDZ. Pure 8YDZ degrades by 40 % (950°C) within thousands of hours due to the decomposition on the nanoscale. Moreover, the degradation of 8YDZ in the presence of Ni proceeds 50 times faster. To clarify this, NiO thin films were deposited onto 8YDZ substrates by electron-beam evaporation. Sintering (1400 °C, 5 h, air) facilitated the incorporation of Ni into the 8YDZ. The influence of annealing under reducing conditions (950 °C) was studied by transmission electron microscopy. The decreased solubility of Ni in 8YDZ under reducing atmosphere led to the nucleation and growth of Ni crystallites within the 8YDZ. Typical chemical variations on the nanoscale after degradation were revealed by analytical TEM techniques (FEI Titan 80-300 microscope). The enhancement of the cation mobility and thus the accelerated decomposition of 8YDZ are explained by the electron capture of dissolved Ni under reducing atmosphere. The strain field due to the increase in size ($r_{Ni^{2+}}$=69 pm, r_{Ni^0}=125 pm) leads to larger displacements of the surrounding ions, which effects the diffusivity of ions in the vicinity of the exsolving Ni.

MM 12.36 Mon 17:30 P5

Theoretical and experimental structure analysis of the (1 0 -1 -1) ZnO twin boundary — •Viktor Hrkac[1], Viola Duppel[2], Yogendra Kumar Mishra[3], Rainer Adelung[3], and Lorenz Kienle[1] — [1]Synthesis and Real Structure, Institute for Materials Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart — [3]Functional Nanomaterials, Institute for Materials Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel

The II-VI semiconductor zinc oxide (ZnO) has been the subject of intensive research due to its wide spectrum of properties which results in a plethora of applications including optoelectronic and piezoelectric technologies. In particular, the morphology and thereby the physical properties of ZnO are significantly affected through defect structures induced by twinning. Thus, a comprehensive understanding of twin interfaces is a pivotal for a future optimization of controlling and device performance. Based on analytical electron microscopic observations, a three dimensional model of the (1 0 -1 -1) twin boundary interface is derived which allows a convincing simulation of experimental micrographs. In addition, dynamic effects at the twin interface can be studied in simulated diffraction patterns via the model. The authors would like to thank the DFG for funding via the SFB 855.

MM 12.37 Mon 17:30 P5

Characterization of Complex Structures by means of Precession Electron Diffraction — Ulrich Schürmann[1], Viola Duppel[2], Saskia Buller[3], Wolfgang Bensch[3], and •Lorenz Kienle[1] — [1]Synthesis and Real Structure, Christian Albrechts University, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [3]Institute of Inorganic Chemistry, Christian Albrechts University, Max-Eyth-Straße. 2, D-24118 Kiel, Germany

Precession electron diffraction (PED) became a versatile tool for the advanced characterization of nanoscaled materials in the last years. The determination of the space group of a material is complicated when applying selected area electron diffraction (SAED) since the zonal and serial reflection conditions are often violated by multiple scattering. This effect can be reduced via PED, so the resulting patterns reflect those which are based on the kinematic approximation. Due to the less dynamic intensity the Laue symmetries and the space groups of the crystals can be determined fast and reliably and enables the ab-initio structure determination of unknown nanoscaled materials. Also the PED gives 3D structural information, e.g. about disorder. An experimental breakthrough related to the PED technique is revealed by the analysis of extremely electron beam sensitive samples like intermetallic phases with melting points around 100 °C. PED is also suitable for the characterization of homologous structures based on variable sequences of building units like in Phase Change Materials (PCM). Financial support by the DFG in the SPP1386 is gratefully acknowledged.

MM 12.38 Mon 17:30 P5

Transmission Electron Microscopy Studies along the Process Chain of Printable Electronics based on Nanoparticulate Systems — •Stefanie Spallek, Benjamin Butz, and Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science, University of Erlangen-

Nuremberg, Germany

Printable electronics based on nanoparticulate systems is a highly active research field due to its enormous economical potential. The goal is to develop routes for fabrication of electronic and optoelectronic devices on flexible substrates by cheap and scalable printing techniques that use inks (or pastes) containing conducting or semiconducting nanoparticles. The performance of the final device critically depends on each step of the process chain which comprises synthesis of the nanoparticles, their functionalization and dispersion to printing pastes, the fabrication of the devices and possible after-treatments. The structural properties that influence the device performance include the shape and size distribution of the nanoparticles after synthesis, their 3D arrangement and interconnection in the functional layers as well as defects that may be introduced at various steps of the fabrication. In this contribution we show several examples of TEM studies along the process chain of printable electronic devices as well as the challenges of the corresponding sample preparation.

MM 12.39 Mon 17:30 P5

Characterization of ex-situ heated Fe70Pd30 thick films using TEM and STEM techniques — •Andriy Lotnyk[1], Christoph Bechtold[2], Burak Erkartal[1], Lorenz Kienle[1], and Eckhard Quandt[2] — [1]Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Inorganic Functional Materials, CAU Kiel, Kaiserstr. 2, 24143 Kiel

The phase transformations in the system Fe-Pd were mostly studied on bulk samples. However, the structural evolutions of Fe-Pd films at the composition of Fe70Pd30 are less examined. Here, Fe70Pd30 films with a thickness of 1-5 micrometer were produced by magnetron sputtering on thermally oxidized Si substrates and on a (001)-oriented MgO substrate. Before deposition, the Si substrates were covered by Au layers for obtaining freestanding films while for the MgO substrate, a Cr/Rh layer was used to enhance epitaxial growth of Fe70Pd30. Polycrystalline bcc Fe70Pd30 films were formed on Si while an epitaxial bct Fe70Pd30 film was grown on MgO. The obtained films were ex-situ heated at 650 °C and at 850 °C for 30 min. After heating of the freestanding bcc Fe70Pd30 film at 650 °C, a film containing the fcc Fe60Pd40 and Fe-rich grains was observed while the transformation from bcc to fcc Fe70Pd30 was found for the films heated at 850 °C. The latter films are decomposing into a Fe-Pd alloy with composition close to 70:30 and Fe-rich precipitates. Heating of the epitaxial bct Fe70Pd30 film at 850 °C also leads to the formation of the fcc structure, however, in this case Fe diffused into MgO and a dissolution of Rh into the Fe70Pd30 phase was observed.

MM 12.40 Mon 17:30 P5

Structural analysis of severly deformed Ni_3Ge — •Andreas Grill, Hans-Peter Karnthaler, and Christian Rentenberger — Physics of nanostructured Materials, University of Vienna, Boltzmanngasse 5, 1090 Wien

Single crystals of the $L1_2$ ordered intermetallic compound Ni_3Ge were severely plastically deformed by high pressure torsion (HPT) and studied by transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron backscattered diffraction and differential scanning calorimetry (DSC). The deformation leads to the formation of nanocrystalline bands (5 to 30 μm wide) that are mainly occurring in regions within 100 μm near the top and bottom surface of the HPT disc. This structural inhomogeneity is shown by SEM images and studied in detail by TEM of focussed ion beam specimens. The analysis shows three different structures occurring next to each other: (i) a highly deformed single crystalline matrix, (ii) a textured nanocrystalline structure inside of the bands and (iii) a nanocrystalline structure with little texture near the surface of the bands in a region of about 3 μm thickness. The grain sizes in the nanocrystalline areas are about 20 nm. The average grade of disordering was investigated by DSC showing an ordering peak at 594 K; with increasing deformation the corresponding values of the enthalpies increase between 10 and 26 J/g. This result agrees with the deformation induced increase of density of bands, that show a much higher degree of disorder than the matrix as resulting from the TEM study.

MM 12.41 Mon 17:30 P5

3D imaging and characterisation of strengthening particles in Inconel 718 using FIB tomography — •Adam Kruk, Adam Gruszczyński, and Aleksandra Czyrska-Filemonowicz — AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Al. A. Mickiewicza 30, 30-059 Kraków, Poland

The Inconel 718 is a commercial nickel-base superalloy, widely used for critical pieces in turbine engines. Its microstructure consists of the γ matrix and strengthening coherent nanoparticles γ' and γ". In the present work FIB tomography technique was used for imaging and characterisation of strengthening particles. FIB tomography is based on a serial sectioning procedure using a FIB/SEM dual beam workstation. Repeated removal of layers as thin as several nm for some hundred times allows to investigate at total a volume of some μm3 with a voxel size as 2.5 nm x 2.5 nm x 2.5 nm. 3D mapping of nanoparticles with high Z-resolution by serial FIB slicing (in a distance of about 2.5 nm) and SEM imaging was performed. Ga ion beam at 30 kV was used to perform a precise in-situ milling. The SEM images at accelerating voltage 1.5 kV were taken with using ESB detector. The real 3D-data of precipitates obtained by FIB tomography, open a new possibility for microstructure analysis of materials for industrial applications.

MM 12.42 Mon 17:30 P5

Analytical transmission electron microscopy investigations of Sn-Pd nanoparticals with core-shell structures — •Dietrich Haeussler[1], Bernhard Schaffer[2,3,4], Fu Liu[1,5], Ferdinand Hofer[4], X. B. Zhang[5], and Wolfgang Jaeger[1] — [1]Microanalysis of Materials, Christian-Albrechts-University Kiel, 24143 Kiel, Germany — [2]SuperSTEM Facility, Daresbury Laboratory, Warrington, WA4 4AD, UK — [3]SUPA, School of Physics and Astronomy, University of Glasgow, UK — [4]Institute for Electron Microscopy, Graz University of Technology, 8010 Graz, Austria — [5]Department of Materials Science and Engineering, Zhejiang University, Hangzhou, 310037, China

Metallic core-shell nanoparticles for applications in catalysis and as data storage materials offer the possibility to tailor macroscopic properties generally not obtained by the single-component particles. We show for Pd-Sn nanoparticles that a combination of the analytical techniques of the spectrum-imaging mode with high-angle annular dark-field imaging in Cs-corrected high-resolution scanning transmission electron microscopy enable to precisely analyse and map structure, morphology, and chemical composition of the particles. Beneficial additional information about the particle structure is obtained from electron nanodiffraction patterns. Our analyses of a number of Sn-Pd particles with diameters as small as 20 nm reveal particles with Pd-rich cores and oxidized shells enriched in Sn as well as polycrystalline alloy particles. The study confirms that these methods are useful for monitoring reactions or degradation for composite nanoparticle materials.

MM 12.43 Mon 17:30 P5

Interface studies on carbon nanotubes grown from $Fe_{20}Ni_{80}$ catalysts particles — •Anja Kiessling, Darius Pohl, Christine Täschner, Mark Herrmann Rümmeli, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, D-01069 Dresden, Germany.

Hard-magnetically terminated carbon nanotubes (CNT) are of particular interest for applications in the field of nanotechnology. Recent results obtained on CNT which are grown from and terminated with FePt nanoparticles [1] imply that there is (i) an enrichment of Pt at the particle surface and (ii) an energetically favored facet from which the carbon is released in order to grow the CNT.

In order to further improve the understanding of the physical principles that govern the catalytic growth of the nanotubes, CNT were grown via plasma-enhanced chemical vapor deposition from Ni-rich $Fe_{20}Ni_{80}$ catalyst particles. Likewise prepared CNT are characterized by means of aberration-corrected high resolution transmission electron microscopy (HRTEM). Particular attention is paid to the question as to whether or not there is an indication for a segregation of one of the alloy constituents to the particle surface, as was previously observed in free FeNi particles of close to equi-atomic composition [2]. It is investigated, if there is a preference for the type of facet from which the CNT grow. For the case of CNT growth from Ni particles, MEAM studies indicate that the (111) facet is energetically favored here [3].

[1] F. Schäffel et al., Appl. Phys. Lett. 94 (2009) 193107/1-3. [2] B. Bieniek et al., J. Nanoparticle Res. (submitted). [3] W. Xiao et al., Surf. Sci. 603 (2009) 1985-1998.

MM 12.44 Mon 17:30 P5

Characterization of Al-Si alloy - TiB2 particles composite structure by STEM — •Justyna Grzonka[1], Tomasz Plocinski[1], Pedro Egizabal[2], and Krzysztof Kurzydlowski[1] — [1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland — [2]TECNALAI Foundation, San Sebastian, Spain

The paper describes results of structural characterization of an Al-Si alloy matrix composite reinforced with TiB2 particles produced by in situ reaction. The properties of such composites, developed for weight reducing and wear resistant applications, critically depend on the inter-phase boundaries between Al-Si alloy matrix and TiB2 particles.

In order to study Al-Si alloy - TiB2 inter-phase boundaries High Resolution Scanning Transmission Electron Microscopy (HRSTEM) was used. Samples representative of the material before and after thermal treatment were prepared using Focused Ion Beam technique (FIB). The Energy Dispersive X-ray Spectroscopy (EDS) was used to map the spatial distribution of the key chemical elements. Phase analyses were performed using X-ray and electron diffraction patterns.

The results of the investigations show that the Si and TiB2 particles do not change with the applied heat treatment. However, other particles appearing in the composite matrix do. In particular, the heat treatment results in formation of Al2O3 and magnesium oxide particles at the inter-phase boundaries between Al alloy and TiB2.

MM 12.45 Mon 17:30 P5

Characterization of Al-Si alloy - TiB2 particles composite structure by STEM — •Tomasz Plocinski[1], Justyna Grzonka[1], Pedro Egizabal[2], and Krzysztof Kurzydlowski[1] — [1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland — [2]INASMET Foundation, San Sebastian, Spain

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MM 12.46 Mon 17:30 P5

TEM diffraction used for 3D profile analysis of nanomaterials — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Nanocrystalline FeAl was made by high pressure torsion deformation of the B2 ordered intermetallic compound Fe-45at.%Al. In this study it is shown that quantitative results for the 3D analysis of bulk nanocrystalline materials can be obtained using profile analysis of selected area diffraction patterns (PASAD). This method allows a quantitative local scale analysis of a wide range of nanomaterials. TEM diffraction patterns showing rings were recorded with a large range of tilting angles ($\pm 52°$ along the shear direction). By applying different tilting angles of the incident beam, the morphology of the nanocrystallites was analysed by using the software PASAD-tools (www.univie.ac.at/pasad). It should be pointed out that because of the strong scattering factor in electron diffraction, the diffraction rings can be recorded in seconds thus allowing to cover a large range of tilting angles in a short time. To compare the results gained from diffraction patterns with those from direct images, TEM samples were cut out of the bulk samples to link them directly to the shear direction and to the shear plane. Both, planar and cross sections of nanocrystalline FeAl were investigated to study the shape and morphology of the nanocrystallites. The 3D reconstruction gained from the images of the different cuts agrees very well with the 3D results gained from the diffraction patterns.

MM 12.47 Mon 17:30 P5

Growth of nanosized ordered domains in nanocrystalline intermetallic FeAl studied by TEM methods — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Severe plastic deformation of intermetallic compounds leads to the formation of a nanocrystalline structure that is frequently accompanied by a loss of the long range order. Up till now this has been monitored by X-ray methods; here it is shown that Transmission Electron Microscopy (TEM) is able to give additional insight. In this study TEM methods are used to reveal that high pressure torsion deformation of FeAl does not lead to a complete destruction of the chemical order B2. It leads to the formation of a structure of a medium range chemical order, composed by nanosized ordered domains of B2 structure (about 2 nm in size). Upon heating the long-range order is recurring by coarsening of the ordered nanodomains until they reach the grain size. The growth of the nanosized ordered domains is studied by using both TEM dark field images and TEM diffraction patterns. The quantitative evaluation of the diffraction ring patterns is carried out with the PASAD method (www.univie.ac.at/pasad). The results deduced from the images and those achieved by PASAD complement each other very well. Furthermore the present example shows that due to the strong scattering factor electron diffraction patterns can be used to evaluate very weak superlattice reflections.

MM 12.48 Mon 17:30 P5

A Method to Locally Determine Layer Dimensions and Interface Roughness for Multilayer Coatings with Ultimate Accuracy — •Dietrich Häussler[1], Ulrich Ross[1], Uwe Heidorn[2], Frank Hertlein[2], Jörg Wiesmann[2], and Wolfgang Jäger[1] — [1]Microanalysis of Materials, Christian-Albrechts-University of Kiel, 24143 Kiel, Germany — [2]Incoatec GmbH, 21502 Geesthacht, Germany

Multilayer coatings consisting of ultrathin bilayers on the nanometer scale are essential components of X-ray optics for advanced X-ray analytical equipment and for synchrotron beamlines. Their functionality is based on X-ray scattering from alternating amorphous layers of materials with differing atomic number Z. The development of those layer systems requires precise monitoring of layer thickness, layer periodicity and uniformity, and of interface quality on different length scales. We describe a method for locally determining layer dimensions and interface roughness of multilayer coatings with ultimate accuracy from intensity profiles obtained from high-angle annular dark-field (HAADF) scanning TEM investigations of multilayer cross-sections. Our procedure allows to obtain separate values for lateral interface roughness and interface broadening. For examples of specially designed W-C multilayer systems it is shown that the layer dimensions can be determined with sub-nanometer precision. Comparisons with spatially averaged data obtained from X-ray reflectivity measurements are in satisfactory agreement with our determination of roughness and layer dimensions. The method fails for heavily disturbed multilayer regions involving growth-induced thickness fluctuations.

MM 12.49 Mon 17:30 P5

Electron holography of Fe nanoparticles embedded in MgO crystals — •Dorin Geiger[1], Hannes Lichte[1], Artem Shalimov[2], and Kay Potzger[2] — [1]Technische Universitaet Dresden, ISP, Triebenberglabor, Zum Triebenberg 50, 01328 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany

In Mg-oxide embedded iron nanoparticles [1] show relevant magnetic fields being epitaxially related to the surrounding matrix. Their properties as nano-dimensional objects can strongly differ from those of the macroscopic ones, due to large surface to volume ratios. They were synthesized by Fe^+ ion implantation at an energy of 100keV (incidence angle 7°) with varying fluences up to 3×10^{17} cm^2. Both alfa-Fe (body centered cubic) and gamma-Fe nanoparticles (face centered cubic) are formed in a surface layer of about 50nm thickness. The content of the alfa-Fe phase, which seems to be responsible for the magnetic behaviour, increases at higher fluences and after annealing [1].

To investigate the magnetic fields at nano-scale, off-axis electron holography was applied using a Cs-corrected transmission electron microscope (Tecnai F20 Cs-corr) [2] working in a pseudo Lorentz mode. This allows the reconstruction of the object wave phase, which can be interpreted quantitatively in terms of electromagnetic fields.

[1] Shalimov, A. et al., Journal of Applied Physics 105, 064906 (2009)
[2] Geiger, D. et al., Microsc. Microanal. (2008) 14, 68-81.

Funding by DFG.

MM 12.50 Mon 17:30 P5

In-situ TEM investigation under extreme heat: Gold and hydrocarbon adsorbates on graphene — •Benedikt Westenfelder[1], Jannik C. Meyer[2], Xiaohang Lin[3], Ferdinand Scholz[1], Carl E. Krill III[4], Axel Gross[3], and Ute Kaiser[2] —

[1]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany — [2]Central Facility of Electron Microscopy, Ulm University, 89081 Ulm, Germany, — [3]Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany — [4]Institute of Micro- and Nanomaterials, Ulm University, 89081 Ulm, Germany

Atomically resolved studies of the heat-induced evolution of adsorbates on graphene have been enabled due to the development of specifically designed TEM sample carriers. Our concept provides to apply in situ an electrical current to a freestanding graphene membrane. In this way we reach local temperatures exceeding 2000 K enabling to observe the transformation of adsorbated hydrocarbons into atomic layers of amorphous carbon and eventually into polycrystalline graphene. Moreover, we observed the migration of gold nanoparticles and their self-organized alignment along parallel straight lines along the negative temperature gradient. Furthermore, we investigated the periodical arrangement of individual gold atoms into rectangularly shaped atomic monolayers and bilayers as well as entire cuboids of many atomic layers. We found, that their lattice parameter is significantly larger than the value for pure gold articles, which might be caused by the incorporation of excess carbon into the gaps of the gold fcc lattice. DFT calculations suggest that an interstitial gold-carbon compound has been developed.

MM 12.51 Mon 17:30 P5

High Resolution Transmission Electron Microscopy of Organic Molecules on Graphene — •Gerardo Algara-Siller[1,2], Goutam Pramanik[3], Tanja Weil[3], and Ute Kaiser[1] — [1]Group of Electron Microscopy of Materials Science, Ulm University, Ulm, Germany — [2]Technical University Ilmenau, Ilmenau, Germany — [3]Department of Organic Chemistry III/Macromolecular Chemistry, Ulm University, Ulm, Germany

Graphene, a one atom thick material, has been proven to be a perfect substrate for TEM investigations. In this work, a graphene substrate was fabricated via micromechanical cleavage and transfered to a Quantifoil grid. In order to reduce contamination on the substrate, graphene was annealed and treated with H2:O2 ion plasma. Solutions of protein based copolymers, cBSA-PEO-TA coated Au nanoparticles (NPs) with different Au-protein ratios were deposited by drop coating on graphene and investigated using an aberration-corrected FEI TITAN 80-300 operated at 80kV acceleration voltage. HRTEM micrographs of the deposited protein based copolymers corroborated that the particle size distribution of the Au NPs is dependant on the Au-protein ratio. Furthermore, due to the low noise graphene substrate, the surrounding protein and single gold atoms forming the NPs can be easily resolved and counted. Thus, we report an approach of lower voltage aberration-corrected HRTEM imaging on graphene towards unraveling the chemistry of inorganic/organic interfaces.

MM 12.52 Mon 17:30 P5

Influence of chemical bonding on HRTEM images of light elements — •Simon Kurasch[1], Jannik C. Meyer[1,3], Hye Jin Park[2], Viera Skakalova[2], Siegmar Roth[2], and Ute Kaiser[1] — [1]Central Facility for Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm — [2]MPI FKF, 70569 Stuttgart — [3]University of Vienna, Department of Physiks, 1090 Vienna, Austria

We improved the HRTEM image simulation by calculating the electrostatic specimen potential via density functional theory (DFT) [1]. This approach takes into account the electron charge redistribution within the specimen due to chemical bonding. Usually this is neglected by calculating the scattering potential as a superposition of isolated atom potentials.

Here we show that chemical bonding is clearly detected in experimental images of nitrogen doped graphene. We found that single atom nitrogen substitutions can be detected in experimental HRTEM images (dZ=1). According to the isolated atom model this should not be possible. However the observation is in excellent agreement with the DFT based simulation. Therefore the observed contrast from the N atom originates from a polarization effect on the neighbouring carbon atoms.

These experiments reveal that bonding has to be included in the TEM image simulation, and that a TEM can be utilized to obtain information about the electronic configuration of the specimen. This opens a way to discern electronic arrangements in point defects or other non-periodic objects that can not be analyzed by diffraction.

MM 12.53 Mon 17:30 P5

The Unitarily Covariant Formulation of Hedin's Equations — •Ronald Starke and Georg Kresse — University of Vienna, Faculty of Physics, Comp Mat Phys

The Feynman graph formulary as used e.g. by Hedin's equations depends on the usage of the spacetime domain. E.g., the well-known GW-approximation is usually formulated as $\Sigma(1,2) = \mathrm{i}G(1,2)W(2,1)$ where $G(1,2)W(2,1)$ denotes a point-wise product in the space time domain, i.e. $1 = x_1 = (\boldsymbol{x}_1, t_1)$. For practical calculations, however, it might be useful to work with quantities given as time (frequency) dependent matrices w.r.t. an orbital basis. The resulting expressions for Σ etc. do not carry over directly from the space-time domain. E.g., $\Sigma^i{}_j \neq \mathrm{i}G^i{}_j W^j{}_i$ already because W is given in an arbitrary orbital basis by a 4-point quantity $W^{ij}{}_{kl}$. It is, therefore, desirable to reformulate Hedin's equations such that they hold in an any orbital basis. In analogy to General Relativity, we call this formulation *unitarily covariant*. For the implementation of such an unitarily covariant formulation, it is necessary to clarify the resulting transformation properties induced by a change of basis in the one-particle Hilbert space $\mathcal{H}$. In particular, it turns out that one has to distinguish between 'upper' and 'lower' indices according to the transformation behavior of the respective quantities. The upshot of the fully covariant formulation will be – apart from a certain theoretical insight – the facilitation of explicit calculation especially when it comes to the derivation of useful approximations: the covariant formalism allows for the direct switch to a basis where certain quantities take particularly simple (e.g. diagonal) forms.

MM 13: HV Motz

Time: Tuesday 10:15–10:45 Location: IFW A

Invited Talk MM 13.1 Tue 10:15 IFW A

Plasticity in confined volumes: new insights into small-scale plasticity — •Christian Motz — Erich Schmid Institute of Material Science, Austrian Academy of Sciences, A-8700 Leoben, Austria

The ongoing miniaturization in many areas of modern technologies, e.g. medical devices, microelectronics, etc., requires material properties in small dimensions. Size effects in mechanical properties prevent the usage of macroscopic material properties. In the last years, it was generally found that there is a specimen size effect on plasticity, i.e. smaller is stronger, if the typical size is reduced to the micrometer regime or below.

3-D discrete dislocation dynamics simulations were performed on samples with sizes from 0.5 to 2 μm to study the size effect and the underlying physical mechanisms. It is shown that the mechanical response strongly depends on the initial dislocation structure and density. For low densities and small samples high flow stresses are observed and the stress vs. strain response shows significant strain bursts. This behaviour is attributed to the inefficiency of generating dislocation sources required for sustained plasticity. For high dislocation densities and/or large samples the flow stress is significantly smaller and a smooth stress vs. strain response is observed. The observed deformation regimes are illustrated in a deformation mechanisms map. Finally, the simulations are compared to experimental data from small-scale experiments, whereas a good agreement is found.

MM 14: Topical Session TEM IV

Time: Tuesday 11:00–13:00 Location: IFW A

Topical Talk MM 14.1 Tue 11:00 IFW A

Transmission Electron Microscopy at 20 kV for Imaging and Spectroscopy - Current Status and Future Prospects — •U. Kaiser[1], J. Biskupek[1], J.C. Meyer[1], J. Leschner[1], L. Lechner[1], Z. Lee[1], S. Kurasch[1], U. Golla-Schindler[1], M. Kinyanjui[1], H. Rose[1], M. Stöger-Pollach[2], A.N. Khlobystov[3], M. Haider[4], P. Hartel[4], H. Müller[4], S. Eyhusen[5], and G. Benner[5] — [1]Central Facility of Electron Microscopy, Ulm University, Germany — [2]USTEM, Vienna University of Technology, Austria — [3]University of Nottingham, United Kingdom — [4]CEOS GmbH, Heidelberg, Germany — [5]Carl Zeiss NTS GmbH, Germany

We demonstrate the feasibility of a transmission electron microscope for direct spatial imaging and spectroscopy using electrons with energy in the range between 20 and 80keV. The highly stable instrument is equipped with an electrostatic monochromator, an imaging energy filter and a CS-corrector. High image contrast is obtained at 20 kV. Using this voltage, we have shown the transfer of the 213 pm lattice structure of single-layer graphene and of the 200 reflections (271.5 pm) of 4 nm thick Si layers. Moreover, radiation-sensitive fullerenes (C60) within a carbon nanotube container withstand at 20kV an about two orders of magnitude higher electron dose than at 80 kV. In spectroscopy mode we show that the quasi-monochromatic low-energy electron beam enables the acquisition of EELS spectra with exceptionally low background noise.

Topical Talk MM 14.2 Tue 11:30 IFW A

Quantification of instrumental properties in high-resolution transmission electron microscopy — •Juri Barthel and Andreas Thust — Institute for Solid State Research and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The precise characterization of the instrumental imaging properties in the form of aberration parameters constitutes an almost universal necessity in quantitative high-resolution transmission electron microscopy, and is underlying most hardware and software techniques established in this field. An effective and reproducible aberration control depends on two crucial aspects: First, an adequate aberration measurement technique is required, which must achieve a sufficient precision depending on the instrumental information limit. Second, an accordingly high optical stability of the microscope is needed, because the relevance of an aberration measurement ends with the lifetime of the measured optical state.

Both prerequisites, measurement precision and instrumental stability, are investigated in a quantitative way with respect to their achievable limits. Numerical procedures are presented for the automatic extraction of the two lower-order aberrations, defocus and 2-fold astigmatism, from single diffractograms of amorphous material [1]. The novel procedures achieve a precision of a nearly 1 Angstrom, which is sufficient to control the optical state and to assess its stability for successful sub- Angstrom microscopy.

[1] J. Barthel, A. Thust, Ultramicroscopy 111 (2010) 27 - 46.

MM 14.3 Tue 12:00 IFW A

Quantitative High-Resolution Transmission Electron Microscopy of Single PlatinumAtoms — •Björn Gamm[1], Radian Popescu[1], Holger Blank[1], Reinhard Schneider[1], Dagmar Gerthsen[1], André Beyer[2], and Armin Gölzhäuser[2] — [1]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Physik Supramolekularer Systeme, Universität Bielefeld, 33501 Bielefeld, Germany

Single atoms can be considered as the most basic objects to be imaged in an electron microscope and can therefore be used to test the image contrast model which comprises the electron-atom interaction and image formation in the microscope. In this work a quantitative comparison of simulated and experimental high-resolution transmission electron microscopy (HRTEM) images of single Pt-atoms is performed to test the basic image contrast model. Single Pt-atoms were deposited on a self-assembled monolayer substrate and imaged by HRTEM using an aberration-corrected microscope. The negligible contrast of the substrate allows the quantification of single-atom contrast. Image simulations are performed on the basis of Weickenmeier-Kohl and Doyle-Turner scattering factors. Objective-lens aberrations as well as the effects of partial coherence and MTF of the CCD camera are considered. The contrast from the simulations is compared with the experimentally measured contrast. Peak intensity and full width at half maximum are determined. For these properties full agreement on an absolute intensity scale is found within the error limits for WK scattering factors.

MM 14.4 Tue 12:15 IFW A

Applications of CS-corrected TEM in metal nitride hard coating materials — •Zaoli Zhang[1], Boriana Roshkava[1], Rostislav Daniel[2], Christian Mitterer[2], Gerhard Dehm[1,2], Petr Lazar[3], Josef Redinger[3], and Raimund Podloucky[4] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences — [2]Department Materials Physics, University of Leoben, Leoben, Austria — [3]Institute of General Physics, Vienna University of Technology, Vienna, Austria — [4]Department of Physical Chemistry, University of Vienna, Vienna, Austria

Using CS-corrected HRTEM), electron energy loss spectroscopy (EELS), and ab-initio density functional theory (DFT) the interface microstructures of VN (CrN)/MgO (001) are closely examined. By HRTEM, we show an atomic resolution structure of epitaxially grown VN film on MgO (CrN/MgO, CrN/Cr/Si) with a clearly resolved oxygen and nitrogen sub-lattice across the interface. As revealed by DFT calculation, the (002) interplanar spacing oscillates in the first several VN layers across the interface. Interfacial chemistry determined by EELS shows the preponderance of O and V atom at the interface of VN/MgO, and V-L2,3 at the interface show a small detectable core-level shift. A clear energy shift of Cr-L2,3 at CrN/Cr/Si interface is observed, Cs-corrected HRTEM images reveal the presence of one interlayer(Cr2N), which leads to the chemical shift of Cr-L2,3.

MM 14.5 Tue 12:30 IFW A

Optimum TEM imaging conditions for graphene at low and medium voltages — •Zhongbo Lee[1], Ute Kaiser[1], Jannik Meyer[2], and Harald Rose[1] — [1]Central Facility of Electron Microscopy, Group of Materials Science Electron Microscopy, University of Ulm, 89069 Ulm, Germany — [2]University of Vienna, Department of Physics, 1090 Vienna, Austria

In standard electron microscopy graphene is usually considered as a weak phase object (WPO) for which the contribution of the non-linear terms to the image contrast is negligibly small. Here we investigate whether this argument holds true for low voltages by means of calculating optimum positive and negative image contrast for an aberration-corrected TEM operating at acceleration voltages of 80kV and 20kV, respectively. The results in the case of achromatic imaging conditions show that graphene cannot be treated as a WPO for low voltages. Even at 80kV the difference between optimum positive and negative contrast is significant. At 20kV this difference becomes very large for the same imaging conditions demonstrating that in this case graphene acts as a strong phase object. In the presence of chromatic aberration, however, the finite energy width of the electron beam largely nullifies this difference. This behavior is shown by the calculations and verified by the experiment for 80kV. Moreover, for chromatic imaging conditions at 80kV the contrast can be increased significantly by means of a monochromator which reduces the energy width to about 0.1eV. In the case of 20kV, however, a significant improvement of contrast can only be achieved by the additional correction of chromatic aberration.

MM 14.6 Tue 12:45 IFW A

Quantitative scanning transmission electron microscopy at low energies — •Erich Müller, Marina Pfaff, Holger Blank, Tobias Volkenandt, Felix Bleimund, and Dagmar Gerthsen — Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany

Sensitive material (Z-)contrast is obtained by high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) at low electron energies ($<$ 30 keV). Even for small atom-number differences, quantitative analysis of composition is possible (e.g. in ternary semiconductors) and the TEM sample thickness can be determined. Moreover, knock-on damage is negligible at low electron energies, which is favorable for the examination of radiation-sensitive materials like semiconductors, organics or biological samples. The electron transmission is measured with a standard annular semiconductor

detector in a state-of-art scanning electron microscope. This allows rapid change of instrumental alignments and parameters like electron energy or collection angles, which is essential for the determination of the characteristic dependence of the image intensity on these parameters. In combination with a focused-ion-beam system, samples with defined geometry and thickness can be prepared from materials with known composition which is essential to test the procedure for the extraction of quantitative image information. The presented method is based on HAADF STEM images and the comparison of the measured intensities with semi-empirical calculations or Monte-Carlo simulations. Examples of radiation-sensitive materials are shown to illustrate the method.

MM 15: Computational Materials Modelling IV

Time: Tuesday 11:00–13:00 Location: IFW B

MM 15.1 Tue 11:00 IFW B

Atomistic Multi-Time-Scale Modelling of Cu-alloyed α-Fe — •David Molnar[1,2], Peter Binkele[1], Stephen Hocker[1], and Siegfried Schmauder[1,2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart — [2]Stuttgart Research Centre for Simulation Technology (SRC SimTech), SimTech Cluster of Excellence, University of Stuttgart

Cu-alloyed α-Fe changes its material behaviour during its ageing process, especially when operated at higher temperatures of above 300°C, due to Cu-precipitates forming on a relatively large time scale within the Fe-matrix. In order to model this complex behaviour, the growth process of precipitates is accounted for by a Kinetic Monte-Carlo (KMC) approach. Several different precipitation states are transferred from KMC as starting configurations to Molecular Dynamics (MD) simulations allowing for nano tensile tests at different stages of the precipitation process and hence at relevant precipitation times. This can be understood as a multi-time-scale approach in a sequential way. Focusing onto single crystals to reveal the sole effect of the precipitates on the mechanical material behaviour, different structural orientations of the α-Fe matrix are investigated in order to obtain an anisotropic temporal behaviour of, e.g., Young's modulus. Thus, the combination of the methods bridges the short time scale of MD with the longer time scale accessible with KMC simulations. In this way, a computational modelling of tensile tests throughout an ageing process of Cu-alloyed α-Fe is achieved as a step towards multiscale-simulation-based design of materials with desired properties.

MM 15.2 Tue 11:15 IFW B

A mesoscale kinetic model for alloys from atomic Monte Carlo simulations — •Thomas Garnier and Maylise Nastar — CEA, Saclay, France

Atomic Kinetic Monte Carlo (AKMC) simulations allow accurate reproduction of diffusion controlled phenomena in alloys when a rigid lattice can be assumed. However, their computational cost limits their scope. On the other hand, if the efficiency of mesoscopic methods like the Phase field method is not in question, their quantitative predictive power is not ensured most of the time. Some progress in improving the accuracy has been recently reported [1]. Following the same procedure [1], we performed Atomic Monte Carlo simulations and measured the composition fluctuation spectrum to determine mesoscopic energy parameters. To take into account the mesh resolution some finite size effects have to be considered. Another usual weakness of the phase field method is the description of the mobilities. AKMC simulations can once again be exploited to obtain the phenomenological transport coefficients associated with a vacancy diffusion mechanism. The resulting energy and kinetic parameters are then used to parameterize a Cellular Monte Carlo method, which is based on a coarse grained description of the alloy. We demonstrate that such an algorithm allows to obtain consistent results for a grid where each point represents from a few to thousands of atoms. Both thermodynamic and kinetic properties remain almost unchanged with the change of scale.

[1] Q. Bronchart & al, Phys. Rev. Lett.,100,015702,(2008)

MM 15.3 Tue 11:30 IFW B

Polyhedron analysis in complex phases — Thomas Schablitzki, •Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The formation of complex phases in metal alloys can significantly influence the macroscopic properties of the material. Topologically close-packed (TCP) phases in Ni-based superalloys, e.g., are brittle and their formation depletes the matrix of refractory elements which leads to a degradation of mechanical properties. The precipitation of Laves phases in steels, on the other hand, improves the strength of the material through precipitation hardening, whereas the formation of σ-phase precipitates has negative effects.

The atomic structure of complex phases is described by an ordered arrangement of coordination polyhedra around inequivalent lattice sites. To identify the corresponding TCP phases during atomistic simulations we have developed a polyhedron analysis. Of particular importance in trying to understand the formation and growth of TCP phases on an atomistic level are processes taking place at the interface between the complex phase and the alloy matrix. Here, we employ an adaptive kinetic Monte Carlo approach together with our polyhedron analysis to investigate concerted atomic rearrangements at the interface.

MM 15.4 Tue 11:45 IFW B

Structure and energetics of nanoclusters in bcc-Fe containing copper, nickel and vacancies — •Ahmed Tamer Al-Motasem[1], Matthias Posselt[2], Frank Bergner[1], and Uwe Birkenheuer[1] — [1]Institute of safety research — [2]Institute of Ion Beam and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

Reactor pressure vessel (RPV) steels consist of polycrystalline bcc-Fe containing Cu, Ni and other foreign atoms. The continuous irradiation by fast neutrons leads to supersaturation of vacancies and self-interstitials and enhances the diffusion of Cu and Ni which occurs via the vacancy mechanism. These processes favor the formation of nanoclusters consisting of vacancies, Cu and Ni. The interaction of dislocations with these precipitates is considered to be the main cause of hardening and embrittlement of the RPV steels. In order to model the evolution of the precipitates under irradiation by rate theory, the energetics and thermodynamics of the clusters must be known. These data are hardly obtainable by experiments, however, they can be provided by atomic-level computer simulations. In the present work a combination of on-lattice Monte Carlo simulations and off-lattice Molecular Dynamics calculations is employed to determine structure and energetics of the nanoclusters. The atomistic simulations show that ternary clusters exhibit a shell structure with a core consisting of vacancies followed by a shell of Cu and an outer shell of Ni. Binary vacancy-Cu and Ni-Cu clusters show a similar shell structure, whereas the atomic configuration of vacancy-Ni agglomerates is completely different.

MM 15.5 Tue 12:00 IFW B

Phase Diagrams from ab-initio calculations: Re-W and Fe-B — •Thomas Hammerschmidt, Arthur Bialon, Mauro Palumbo, Suzana G. Fries, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The CALPHAD (CALculation of PHAse Diagrams) method relies on Gibbs energy databases and is of limited predictive power in cases where only limited experimental data is available for constructing the Gibbs energy databases. This is problematic for, e.g., the calculation of the phase transformation kinetics within phase field simulations that not only require the thermodynamic equilibrium data but also information on metastable phases. Such information is difficult to obtain directly from experiment but ab-initio calculations may supplement experimental databases as they comprise metastable phases and arbitrary chemical compositions. We present simulations for two prototypical systems: Re-W and Fe-B. For both systems we calculate the heat of formation for an extensive set of structures using ab-initio calculations and employ the total energies in CALPHAD in order to determine the corresponding phase diagrams. We account for the configurational entropy within the Bragg-Williams approximation and neglect the phenomenological excess-term that is commonly used in CALPHAD as well as the contribution of phonons and electronic excitations to the free energy. According to our calculations the complex intermetallic phases in Re-W are stabilized by the configurational entropy. For Fe-B, we calculate metastable and stable phase diagrams including recently

predicted new stable phases.

MM 15.6 Tue 12:15 IFW B

Atom probe tomography as a tool to determine binding energies in Cu_3Au — •Torben Boll[1,2], Talaat Al-Kassab[1,2], Zhiyong Zhu[1], and Udo Schwingenschlögl[1] — [1]Division of Physical Sciences and Engineering King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Binding energies are important parameters for many material properties. In this paper simulations and experimental results of atom probe tomography data for $L1_2$-Cu_3Au will be presented. An important parameter in the simulations is the binding between the different species. A (12,6)-Lennard-Jones potential is assumed to govern the binding and thus the evaporation process, which is modeled according to the Müller-Schottky theorem. By adjusting the Cu-Au-binding potential of the simulation to fit the experimental results a very good agreement can be reached.

The conclusion is supported by simulations and experiments for the <220> and <200> crystallographic superstructure and the <111> non-superstructure directions.

For comparison a density functional theory method was applied to determine the binding energies. The findings further support our APT-based approach.

MM 15.7 Tue 12:30 IFW B

Effect of uniaxial loading on the structural anisotropy and the dynamics of atoms of Cu-Zr metallic glasses within the elastic regime studied by molecular dynamic simulation — •Yue Zhang[1], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The changes in the structure and the dynamics of atoms and the stress-induced structural anisotropy of a Cu50Zr50 metallic glass upon the application of uniaxial compressive and tensile stresses within the elastic regime during the loading and unloading processes have been studied using molecular dynamic simulation. It is found that the structural change is more significant under tension than under compression, which is accompanied with the destruction of the full icosahedra clusters into distorted ones. Permanent structural change is found at the applied tensile stress of 1000 MPa but still within the elastic regime. The structural anisotropy increases monotonously with the applied stress, being more pronounced along the loading direction than the other two free directions. The results of the mean square displacement, the non-gaussian parameter and the mobile atom analysis suggest that the dynamics of the atoms is distinctly different under uniaxial stresses above 800 MPa. The permanent change in the structure and structural anisotropy can be correlated with the change in the dynamics of the atoms.

MM 15.8 Tue 12:45 IFW B

Investigations of charge and energy distributions in electron beam induced deposition of tungsten — •Harald O. Jeschke, Carlos Ortiz, and Roser Valentí — Institut für Theoretische Physik, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

We employ Monte Carlo simulations of particle trajectories to study the irradiation of a SiO_2 substrate and a $W_xC_yO_z$ deposit with a 5 keV electron beam. We determine the energy distribution of backscattered electrons which is important for the fragmentation of adsorbed $W(CO)_6$ precursor molecules. We also study the distribution of positive and negative charges in deposit and substrate as function of depth and radial distance from the beam center in a cylindrical geometry. Finally, we determine the profiles of the deposited energy which lead to nonequilibrium electron distributions. We relate our findings to experimental observations.

MM 16: Structural Materials

Time: Tuesday 11:00–13:00 Location: IFW D

MM 16.1 Tue 11:00 IFW D

Temperature dependent lattice misfit in Nickel-base superalloys - Simulation and experiment — •Steffen Neumeier and Mathias Göken — Lehrstühl für Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg, Erlangen, Deutschland

Ni-base superalloys are widely used in high temperature applications like jet engines and land-based turbines, because of their excellent high temperature properties. They derive their excellent high temperature strength and creep resistance from the presence of a high volume fraction of Ni_3Al γ' precipitates ($L1_2$ structure), which are embedded coherently within the face centred cubic (A1) γ matrix. The magnitude and sign of the lattice misfit between γ and γ' are important parameters affecting the microstructural evolution and high temperature strength of Ni-base superalloys. Therefore the knowledge of the lattice misfit at application temperature is of great importance. In this study the lattice misfit of several 1^{st}, 2^{nd} and 4^{th} generation Ni-base superalloys in dependence of temperature has been measured by means of HRXRD and compared with lattice misfit simulations based on thermodynamic calculations. The influence of the thermal expansion coefficients and the change in the chemical composition of both γ and γ' due to the γ' dissolution with increasing temperature has been taking into account. The experimentally measured γ and γ' lattice parameters could be reproduced by the simulation and the γ/γ' lattice misfit could be reasonably predicted.

MM 16.2 Tue 11:15 IFW D

Short-range order in Ni-rich Ni-W alloys investigated by synchrotron measurements and first-principles calculations — •Nils Schindzielorz[1], Sascha Maisel[1], Alexey Bosak[2], Harald Reichert[2], and Stefan Müller[1] — [1]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg — [2]European Synchrotron Radiation Source (ESRF), 6 Rue Jules Horowitz, F-38043 Grenoble

Ni-rich Ni-W alloys show a whole zoo of short-range order phenomena as observed by diffuse X-ray scattering. It will be shown that the quantitative analysis of these patterns can be successfully performed by the combination of X-ray scattering and ab-initio based calculations. For the latter, the combination of density functional theory with the cluster expansion method as realized in the computer code UNCLE and Monte-Carlo simulations is applied. This allows us to predict the short-range order in real and k-space as a function of concentration and temperature. The predicted patters are compared with experimental data. It turns out that the short-range order in Ni-W can only be explained by the simultaneous existence of different structure types, where the D16 compound plays one important role.

MM 16.3 Tue 11:30 IFW D

Energetics of TiAlNb alloys with interstitial carbon — •Dominik Legut[1,2], Juergen Spitaler[1,2], Pasquale Pavone[1,2], and Claudia Ambrosch-Draxl[1] — [1]Atomistic Modelling and Design of Materials, Leoben, Austria — [2]Materials Center Leoben, Leoben, Austria

TiAl based alloys exhibit attractive properties such as low density, high strength at high temperatures, and very good oxidation resistance. However, they are brittle at room temperature. It was recently found that lamellar structures, obtained by alternating the γ and α_2 phase, addition of transitional metal or interstitial elements like carbon increase ductility and creep strength at room temperature.

We perform first-principles calculations based on density-functional theory to study the influence of interstitial carbon on the energetics of both the γ and α_2 phase of the TiAlNb alloy system, where Nb atoms substitute Ti sites. In particular, we determine the heats of formation with respect to the pure TiAl phases, taking into account various configurations for the substitutional Nb sites. In our calculations, the carbon atoms are located on one of two possible interstitial sites.

We consider two different situations. First, Al-rich systems are obtained by replacing Ti atoms with Nb. Second, in Ti-rich systems, the concentration of Ti atoms is kept constant (50%) by moving the Ti atoms replaced by Nb to Al sites. We find that in all cases the energy cost of accommodating carbon is very much affected by the presence of the alloying element Nb.

MM 16.4 Tue 11:45 IFW D

First principles study of elastic properties of eutectic Ti-Fe alloys up to their mechanical stability limits — •Li-Fang Zhu, Martin Friák, Alexey Dick, Alexander Udyansky, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

Ti-based alloys have been suggested for commercial applications due to their high strength and good corrosion resistance. Motivated by experimental results showing eutectic Fe-Ti alloys decomposing into the FeTi compound with B2 structure and beta-Ti(Fe) alloys with varying Ti concentration (depending on the cooling rate), Ti-Fe alloys covering a broad range of Ti concentrations were studied using density functional theory (DFT) within the generalized gradient approximation (GGA). After examining thermodynamic stability and structural properties, ground-state single crystalline elastic constants have been calculated and homogenized in order to determine experimentally accessible elastic moduli. Employing the quasi-harmonic approximation, temperature dependences of single-crystaline and polycrystalline elasticity parameters have been predicted. Further, by simulating tensile tests along [001], [110] and [111] directions, the theoretical tensile strengths have been determined for both FeTi-B2 and beta-Ti(Fe) phases. In addition, the brittle-fracture crystal separation was simulated for (001), (110) and (111) planes. Searching for a loading mode of materials failure, our FeTi-B2 results show that the theoretical tensile strength is lowest along the [001] direction and that the brittle-fracture crystal separation energy is lowest for the (110) plane.

MM 16.5 Tue 12:00 IFW D

Ultra fast in situ hard X-rays micro-tomography: Application to solidification and hot tearing of alloys or heat treatment of super conductors — •Mario Scheel[1], Marco Di Michiel[1], Luc Salvo[2], Pierre Lhuissier[2], Bastien Mireux[2], Michel Suéry[2], and Christian Scheuerlein[3] — [1]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France — [2]Laboratoire SIMAP - Groupe GPM2, BP 46 Saint Martin d'hères, France — [3]European Organization for Nuclear Research (CERN), TE-MSC, Geneva, Switzerland

Hard X-rays micro-tomography allows getting 3D images with spatial resolution in the micron range in a non-destructive manner. It has been applied now in a wide range of research fields (damage in materials, foams, solidification, etc.). Thanks to the high flux of synchrotron and ultra fast cameras the total time to acquire a scan was considerably reduced. The use of specific devices mounted (furnaces, tensile compression machine) allows performing in situ tomography on various materials. We performed 3D in situ solidification of aluminium-copper alloys at fast cooling rates (between 1 to 10°C/s) and we will show results on the early stage of solidification (morphology of solid phase, kinetics of growth). In addition the formation of porosity and the phase evolution during the reaction heat treatment of superconducting wires has been monitored.

MM 16.6 Tue 12:15 IFW D

Conical slits for depth-resolved stress measurements with high-energy X-rays — •Torben Fischer, Peter Staron, Eike-Henning Eims, Sebastian Frömbgen, Norbert Schell, Martin Müller, and Andreas Schreyer — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Geesthacht, Germany

The use of photons with energies from about 50 keV up to about 150 keV and the resulting large penetration depths enables diffraction measurements in the bulk of the material and, thus, to obtain information e.g. on residual stresses even within larger components. The depth resolution that is required for such measurements can be achieved by the use of a conical slit system in the case of monochromatic radiation. Such a system was tested at the new high-energy material science beamline HEMS of the Helmholtz-Zentrum Geesthacht at the new PETRA III synchrotron at DESY, Hamburg. The samples used for the test were laser beam welded (LBW) steel sheets. The LBW technique is currently still being developed for applications in civil aircraft production and automotive industry for reducing weight and production costs. The LBW introduces residual stresses in the weld and heat affected zone. These stresses can have disadvantageous influence on the service performance of the weld. LBW overlap joints of DC04 steel with a thickness of 2 mm were investigated by this technique and the results were compared with the results of neutron diffraction measurements.

MM 16.7 Tue 12:30 IFW D

***In situ* investigation of friction stir welded AA7449 using high energy SAXS** — •Malte Blankenburg, Torben Fischer, Peter Staron, Luciano Bergmann, Jakob Hilgert, Jorge F. dos Santos, Martin Müller, and Andreas Schreyer — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Strasse 1, 21502 Geesthacht, Germany

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

The intermediate stages of precipitation or phase transformations in the weld zone during the joining process can only be registered by *in situ* experiments. The transportable FSW system 'FlexiStir' developed at HZG provides the opportunity to perform *in situ* small-angle X-ray scattering (SAXS) experiments during FSW. So far, FlexiStir was used at the HZG high energy synchrotron beamline HARWI II at HASYLAB. As a result, spatial resolved size and volume fraction distributions of precipitates in the heat affected zone during the FSW process were obtained.

MM 16.8 Tue 12:45 IFW D

Light weight metal compounds with ultra-fine grained microstructure — •Tom Marr[1,2], Jens Freudenberger[2], Juliane Scharnweber[1], Carl-Georg Oertel[1], Werner Skrotzki[1], Uwe Siegel[2], Uta Kühn[2], Jürgen Eckert[2], Ulrich Martin[3], and Ludwig Schultz[1,2] — [1]TU Dresden — [2]IFW Dresden — [3]TU Bergakademie Freiberg

Composites of titanium and aluminium have been severely plastically deformed using a repetitive bundling and swaging technique. This process allows to reaching high logarithmic deformation strains. In consequence, an ultra-fine grained microstructure of all phases is observed, resulting in a high specific strength, making this materials suitable for constructive applications. Among these composites, ultimate tensile strengths of around 800 to 900 MPa are reached in combination with a final mass density of 3-4 g/cm^3.

MM 17: Topical Session TEM V

Time: Tuesday 14:00–15:30 Location: IFW A

Topical Talk MM 17.1 Tue 14:00 IFW A

New Electrostatic Phase Plate for Phase-Contrast Transmission Electron Microscopy and Its Application for Wave-Function Reconstruction — Björn Gamm[1], Katrin Schultheiss[2,4], Joachim Zach[3], Manuel Dries[1], Nicole Frindt[4], Rasmus R. Schröder[4], and •Dagmar Gerthsen[1] — [1]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Germany — [2]InnovationLab, Speyerer Straße 4, 69115 Heidelberg, Germany — [3]CEOS GmbH, Englerstr. 28, 69126 Heidelberg, Germany — [4]Bioquant Cell Networks, Universität Heidelberg, 69120 Heidelberg, Germany

We present a promising new design of an electrostatic physical phase plate for transmission electron microscopy. The design consists of a microcoaxial cable with the exposed electrode positioned near the undiffracted beam in the back focal plane of the objective lens. The absence of an obstructing ring electrode around the central beam overcomes the major drawback of Boersch-type phase plates. The new phase plate was used to acquire phase-contrast images with different phase shifts of the undiffracted electrons. These images are used to reconstruct the complex image wave function. After correction for the

objective-lens aberrations the object-wave function is obtained, which contains information as for example phase shifts due to the differences of the mean inner potential. The reconstruction algorithm is demonstrated for experimental images from platinum nanoparticles.

MM 17.2 Tue 14:30 IFW A

2D interband plasmons in free-standing graphene — •Michael Kinyanjui[1], Philipp Wachsmuth[1], Jannik Meyer[2], Christian Kramberger[2], Thomas Pichler[2], Gerd Benner[3], and Ute Kaiser[1] — [1]Central facility of electron microscopy, University of Ulm, Albert Einstein Allee 11, 89068 Ulm, Germany — [2]Faculty of physics, University of Vienna, Strudlhofgasse 4, A-1090 Vienna, Austria — [3]Carl Zeiss NTS GmbH, Carl-Zeiss-Str. 56 73447, Oberkochen, Germany

Due to its unique electronic structure 2 dimensional (2D) graphene offers a means by which many-body interactions such quasi-particle excitations (electron-hole pair interactions), collective excitations of valence electrons (plasmons) and lattice vibrations (phonons) can be studied [1]. We investigated the properties of the π-plasmon excitations in free-standing monolayer of graphene using electron energy loss spectroscopy (EELS). The investigations were conducted at a specially developed low voltage transmission electron microscope operated at 20 kV. We study the dispersion of the π Plasmon peak for momentum transfers 0 Å-1 $<$ q $<$ 0.5 Å-1. In this momentum transfer range we observe the π plasmon as being characterized by a quasi-linear dispersion. In addition, the π plasmon excitations are shown to lie above the single-particle excitations (SPE) in mono-layer graphene. These results are discussed and compared to results obtained from single-walled carbon nanotubes (SWCNT).

[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K.S. Novosolev, A. K. Geim, Rev. Mod. Phys. 81, 109 (2009)

MM 17.3 Tue 14:45 IFW A

Inelastic Electron holography : First results with surface plasmons — •Roeder Falk and Lichte Hannes — Triebenberg Labor, Institute for Structure Physics, TU Dresden, 01062 Dresden, Germany

Inelastic interaction and wave optics seem to be incompatible in that inelastic processes destroy coherence, which is the fundamental requirement for holography. In special experiments it is shown that energy transfer larger than some undoubtedly destroys coherence of the inelastic electron with the elastic remainder. Consequently, the usual inelastic processes, such as phonon-, plasmon- or inner shell-excitations with energy transfer of several out to several , certainly produce incoherence with the elastic ones. However, it turned out that within the inelastic wave, *newborn* by the inelastic process, there is a sufficiently wide area of coherence for generating *inelastic holograms*. This is exploited to create holograms with electrons scattered at surface-plasmons, which opens up quantum mechanical investigation of these inelastic processes. P.L. Potapov, H. Lichte, J. Verbeeck and D. van Dyck, Ultramicroscopy 106(2006) 1012. These investigations have been performed within European Union Framework 6, Integrated Infrastructure, Reference 026019 ESTEEM.

MM 17.4 Tue 15:00 IFW A

FIB Target preparation for 20 kV T(S)EM - A method for obtaining ultra-thin lamellas — •Lorenz Lechner, Johannes Biskupek, and Ute Kaiser — Center for Electron Microscopy, Materials Science Group, Ulm University, Ulm, Germany

Recently, scientists have rediscovered the advantages of using low energies in transmission electron microscopy (TEM). It dramatically reduces knock-on damage for imaging low-Z number material and enables electron energy loss spectroscopy up to very high energy losses with exceptionally low background noise. Alas, low voltage TEM requires extremely thin specimens free of preparation artifacts. Conventional focused ion beam (FIB) preparation methods cannot be employed to create high quality specimens much thinner than 25 nm. We have developed a new method for in-situ target preparation of ultra-thin TEM lamellas by FIB milling. With this method we are able to routinely obtain large area co-planar lamellas thinner than 10 nm. The resulting specimens are suitable for low kV TEM as well as transmission scanning electron microscopy (tSEM). We have demonstrated atomic resolution using Cs-corrected TEM at 20 kV on a so prepared Si specimen only 4 nm thick.

MM 17.5 Tue 15:15 IFW A

Site and orientation specific FIB preparation technique for TEM investigation of individual nanostructures, organic thin films and sensitive materials — •Benito Fernando Vieweg and Erdmann Spiecker — CENEM, University of Erlangen-Nürnberg

Sample preparation is a crucial step for analytical and high-resolution transmission electron microscopy (TEM). While conventional techniques, like mechanical thinning followed by low-voltage Ar ion beam milling, have been optimized for preparation of high-quality samples, there are many challenges which cannot be addressed by these techniques. For instance, TEM investigation of individual anisotropic nanostructures in a predefined cross-section orientation requires site and orientation specific preparation which can only be addressed by focused ion beam (FIB) techniques. Common techniques (H-bar, lift-out) require a protective coating, which may alter the surface and degrade the observation of the nanostructure during FIB milling. Sensitive materials like organic thin films or biological materials may as well be altered by the protective coating and are furthermore sensitive to the Ga ion beam. Cross sections of such materials or devices are indispensable for chemical and microstructural analysis, however.

In this contribution an advanced FIB-preparation method is presented which does not require the deposition of a protective coating and furthermore minimizes the impact of the Ga ion beam on the material. Various applications will be presented, including the cross-sectioning of metal nanorods, organic thin film devices and scales of butterfly wings and their investigation by analytical and high-resolution TEM.

MM 18: Mechanical Properties I

Time: Tuesday 14:00–15:30 Location: IFW B

MM 18.1 Tue 14:00 IFW B

Mechanical properties and plastic anisotropy of aluminium laminates produced by accumulative roll bonding (ARB) — •Paul Chekhonin[1], Benoit Beausir[1], Juliane Scharnweber[1], Carl-Georg Oertel[1], Werner Skrotzki[1], Heinz Werner Höppel[2], and Jörn Jaschinski[3] — [1]Institut für Strukturphysik, Technische Universität Dresden — [2]Lehrstuhl Allgemeine Werkstoffwissenschaften, Universität Erlangen-Nürnberg — [3]Institut für Leichtbau und Kunststofftechnik, Technische Universität Dresden

Aluminium sheets with layers of different purity (99.999 and 99.5) have been produced by ARB. The tensile strength and Lankford parameter as a function of the number of ARB cycles are measured by tensile testing. ARB increases the tensile strength significantly. The planar anisotropy decreases with the number of ARB cycles while the normal anisotropy reaches a plateau after 2 cycles. The results will be compared with those of ARB aluminium with a purity of 99.5.

MM 18.2 Tue 14:15 IFW B

Inhomogeneity of texture and microstructure in copper deformed by ECAP — •Christine Tränkner, Robert Chulist, Benoit Beausir, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

Polycrystalline copper of high purity was deformed by equal channel angular pressing (ECAP) at room temperature using routes A, B_C and C with up to 4 passes. Local textures were measured by high-energy synchrotron radiation. For route B_C this was done along 3 lines in the cross section from the top to the bottom of the billets; for routes A and C along 1 line in the middle of the cross section. Using orientation imaging by electron backscatter diffraction microstructure analysis was performed in the cross and in the longitudinal section.

Texture gradients in normal direction of the billets were found for all routes, while in addition a texture gradient in transverse direction was found for route B_C. The texture is compared with that of simple shear. Different microstructures for route A, B_C and C were detected in the cross and in the longitudinal section. They are presented for 4 passes and discussed with regard to the change of shear plane position

when rotating the sample between two passes. The average grain size after 4 passes is approximately 1 μm for all routes. Grain refinement is explained by continuous dynamic recrystallization.

MM 18.3 Tue 14:30 IFW B

Shear band formation in sub-microcrystalline Ni — •Benoit Beausir[1], Lutz Hollang[1], Suhash Ranjan Dey[2], Ellen Hieckmann[3], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, Indian Institute of Technology Hyderabad, Ordnance Factory Estate, Yeddumailaram-502205, Andhra Pradesh, India — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany

The stability of sub-microcrystalline nickel produced by pulsed electrodeposition without any additives was investigated during cyclic deformation at very high plastic strain amplitude of 1% at room temperature. The initial microstructure having an average grain size of 160 nm in the growth plane and a weak <110> fibre texture along the growth direction undergoes considerable grain growth during cyclic loading without significant changes in texture. After a certain number of loading cycles the specimen suddenly developed a single macro shear band. The shear band appeared in the tensile half cycle under 45° to the loading axis and acts as crack starter. Investigations in the scanning electron microscope using electron backscatter diffraction revealed that the main macro shear band consists of relaxed grains elongated along the shear plane displaying a texture induced by shear. The texture in the shear band was reproduced with the viscoplastic self-consistent polycrystal model using {111}<110> slip systems. Detailed investigations of the surrounding of the macro shear band reveal the existence of a large number of regularly spaced micro shear bands.

MM 18.4 Tue 14:45 IFW B

Properties of non-equilibrium grain boundaries in UFG nickel produced by severe plastic deformation — •Gerrit Reglitz, Sergiy Divinski, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Ultra-fine grained (UFG) materials produced by severe plastic deformation (SPD) have become an important target of research due to their improved properties and the promise they hold with respect to novel applications. It has been suggested by several authors that so-called non-equilibrium grain boundaries in SPD processed materials are largely responsible for their properties. These non-equilibrium grain boundaries contain a high density of extrinsic (excess) dislocations and an increased excess free volume. The existence and the properties of non-equilibrium grain boundaries can be studied in great detail by grain boundary diffusion measurements, because such non-equilibrium grain boundaries should represent ultra-fast diffusion paths in comparison to conventional, relaxed high-angle grain boundaries in coarse grained materials.

Grain boundary self-diffusion in UFG Ni prepared by Equal Channel Angular Pressing (ECAP) has been measured by applying the 63Ni radioisotope in combination with the parallel sectioning technique. The results indicate the existence of ultra-fast diffusion paths. The influence of the ECAP processing parameters will be presented. The origin of the ultra-fast diffusion pathways and their possible relation to non-equilibrium grain boundaries will be discussed.

MM 18.5 Tue 15:00 IFW B

Controlling the strength of nanocrystalline metals and alloys: On the role of the grain boundary relaxation state — •Jonathan Schäfer, Alexander Stukowski, and Karsten Albe — TU Darmstadt, Darmstadt, Germany

Plastic deformation in various nanocrystalline metals and their alloys is studied by means of atomic scale computer simulations.

The distribution of solutes is equilibrated in nanocrystalline model structures of different grain sizes and compositions using a combination of Monte-Carlo and molecular dynamics methods. The resulting samples are deformed under uniaxial load. The role of grain boundary relaxation is analyzed in detail by comparing chemically and structurally relaxed samples with model structures that were only structurally relaxed. The relaxation state of the grain boundary is measured by means of the atomic free volume. The defect evolution within the grains of our nanocrystalline model structures is monitored, using a novel dislocation extraction algorithm.

The main goal of this work is to make a connection between the atomistic configuration within the microstructures and the characteristics of the observed stress-strain behaviour.

The simulations reveal that the relaxation state of the GBs is of great importance for the maximum strength in the case of all studied material systems and grain sizes. The (chemical) equilibration is proven to raise the barrier for GB mediated processes. Also in the case of grain sizes, where the major carrier of plastic deformation is dislocation slip, the relaxation state of the GB is shown to have a significant effect.

MM 18.6 Tue 15:15 IFW B

Tilings as models for auxetic cellular structures — •Holger Mitschke[1], Jan Schwerdtfeger[2], Vanessa Robins[3], Carolin Körner[2], Robert F. Singer[2], Klaus Mecke[1], and Gerd E. Schröder-Turk[1] — [1]Theoretische Physik I, Universität Erlangen-Nürnberg — [2]Insitute of Advanced Materials and Processes, University of Erlangen-Nuremberg — [3]Applied Maths, School of Physical Sciences, Australian National University, Australia

In most auxetic materials, the negative Poisson's ratio is a consequence of the geometry of the microstructure. This motivates the search for auxetic structures in archives of mathematical models, such as planar tiling or spatial periodic networks. Here we study the deformation of planar tilings, interpreted as skeletal structures. Our numerical study of their deformations reveals several new auxetic structures and examples with different degrees of freedom, i.e. rigid, unique-flexible or flexible with several deformation modes. In the latter case, we show that the conservation of initial symmetries are a possibility to enforce a unique deformation corresponding to the energy minimum of an energy functional, e.g. given by harmonic angular springs at the vertices. Furthermore we show that elastic cellular structures, built by Ti-6Al-4V selective electron-beam melting rapid prototyping precisely on the basis of the newly found auxetic skeletal structures, possess the same deformation behaviour, namely a negative Poisson's ratio. Finally, the analysis of repositories of three-dimensional tilings or networks (such as `www.epinet.anu.edu`) is equally possible and has the potential to yield conceptually new truly-3D auxetic deformation mechanisms.

MM 19: Transport

Time: Tuesday 14:00–15:30 Location: IFW D

MM 19.1 Tue 14:00 IFW D

Transport and magnetic properties of non-stochiometric FeSi — Monika Kotzian, Tommy Reimann, Dirk Schulze Grachtrup, Stefan Süllow, and •Dirk Menzel — Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

Although the narrow-gap semiconductor FeSi has a non-magnetic ground state, it shows a residual Curie-like susceptibility at low temperature. Whereas this Curie-tail was generally attributed to a surplus of Fe^{3+}, magnetic measurements imply that the residual susceptibility of samples with a slight Fe deficit is larger compared to samples with Fe excess. The transport properties of off-stochiometric tri-arc Czochralski-grown FeSi crystals have been investigated. The temperature dependence of the conductivity suggests that Anderson-localized states which stem from structural disorder carry the residual magnetic moment. Magnetoresistance measurements, which give some indications for a weakly localized system, support this interpretation. In addition, within an impurity model they show that the number of such localized states in the off-stochiometric samples is larger for Fe deficit than for Fe excess. Annealing experiments reveal that the off-stochiometry has a larger influence on the magnetic and transport properties than the presence of crystalline imperfections.

MM 19.2 Tue 14:15 IFW D

Fast grain boundary self-diffusion in ultrafine grained Ag produced by equal channel angular pressing — •Jochen Michael Fiebig[1], Werner Skrotzki[2], Sergiy V. Divinski[1], Mar-

tin Peterlechner[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms Universität, 48149 Münster — [2]Institut für Strukturphysik, Technische Universität Dresden

We performed a systematic study of grain boundary self-diffusion in ultrafine grained silver produced by equal channel angular pressing (ECAP) using samples deformed up to 3 passes according to route A. The resulting ultra-fine grained microstructure was studied by transmission electron microscopy and electron backscatter diffraction. The radiotracer method (^{110m}Ag-tracer solution) in combination with parallel sectioning by microtome slicing was used to obtain the diffusion properties. The activity of each section was counted by a high-purity Ge detector. 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. so-called *non-equilibrium* grain boundaries. Percolating porosity, as already observed for Cu and Cu-alloys produced by ECAP also exists in ECAP-Ag. Applying Borisov's formalism the excess energy of non-equilibrium 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 non-equilibrium grain boundaries is about 10% to 15% higher.

MM 19.3 Tue 14:30 IFW D

Grain Boundary Diffusion in Ultra Fine Grained Copper Produced by High Pressure Torsion — •Matthias Wegner[1], Jörn Leuthold[1], Martin Peterlechner[1], Daria Setman[2], Michael Zehetbauer[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, D-48149 Münster, Germany — [2]Physics of Nanostructured Materials, University of Vienna, A-1090 Wien, Austria

Short-circuit diffusion paths in Ultra Fine Grained copper produced by High Pressure Torsion (HPT) are investigated by the radiotracer method. *Ultra fast* diffusion in addition to conventional grain boundary diffusion is observed. This feature might be related to the existence of so called Non Equilibrium Grain Boundaries (NEGBs) acting as ultra fast diffusion paths. According to the existing models of grain refinement by severe plastic deformation (as e.g. HPT), the abundance of lattice dislocations created during the severe straining serves to modify the grain boundary structure of high angle grain boundaries such that NEGBs with enhanced excess free energy densities are created. The kinetics and structural properties of NEGBs are thoroughly investigated. Furthermore, a network of percolating porosity introduced during the HPT process is observed. This unexpected feature is investigated utilizing the radiotracer technique. A strong dependence of the effective diffusivity and the volume fraction of the porosity on the applied quasi-hydrostatic pressure during HPT is elucidated.

MM 19.4 Tue 14:45 IFW D

Diffusion in a Cu bicrystal with near $\Sigma5$ grain boundary — •Henning Edelhoff[1], Sergej Prokofjev[2], Sergij Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Moscow region, Russia

For the overall understanding of kinetic processes along grain boundaries of polycrystalline and nanocrystalline materials it is essential to understand the processes in a single, well defined grain boundary. In this work, for the first time, the grain boundary diffusion of a solute is measured in a single grain boundary in the C kinetics regime according to the common Harrison classification. The radiotracer technique in combination with parallel sectioning by microtome is used to determine ^{110m}Ag diffusion rates in Cu $\Sigma5$ (310) [001] bicrystal along and perpendicular to the <001> misorientation axis under formal conditions of the B-type and C-type regime.

These studies provided in the B-type regime the values of the triple product $P = s \cdot d \cdot D_{gb}$ of the segregation coefficient s, the effective (diffusional) grain boundary width d and the grain boundary diffusion coefficient D_{gb}, with the latter being directly determined in the C-type regime. A moderate but measurable anisotropy of the grain boundary diffusion is established. The anisotropy of the product $s \cdot d$, which could be related to a heterogeneous segregation of Ag in the grain boundary, is estimated.

MM 19.5 Tue 15:00 IFW D

Recent advances in grain boundary diffusion studies — •Sergiy Divinski — Institute of Materials Physics, University of Münster

A short overview of a recent progress in experimental investigation of grain boundary diffusion and segregation phenomena is presented. The talk is focused on solute diffusion in bi- and tri-crystals. Using the radiotracer technique in combination with serial sectioning and applying precisely characterized bicrystals, the grain boundary diffusion was for the first time measured at low temperatures under the C kinetic conditions [1] after common Harrison's classification. The anisotropy of the grain boundary diffusion coefficient, D_{gb}, and that of the triple product P, $P = s \cdot \delta \cdot D_{gb}$, was measured for Ag diffusion in Cu near $\Sigma5$ grain boundary. The data are discussed in relation to the grain boundary structure.
The first measurements of Ag diffusion along a triple line in tri-crystal [2] are presented and discussed with respect to the triple line energy.
1. H. Edelhoff, S.I. Prokofjev, S.V. Divinski, Scr. Mater. (2010) doi: 10.1016 j.scriptamat.2010.10.032
2. S.V. Divinski, H. Edelhoff, G. Gottstein, L.S. Shvindlerman, B. Zhao, to be published.

MM 19.6 Tue 15:15 IFW D

Study of 44Ti grain boundary self-diffusion in thin nanocrystalline TiO2 films — •Petr Straumal[1,2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, D-48149 Muenster, Germany — [2]National University of Science and Technology "MISIS", 119049 Moscow, Russia

Titanium dioxide is known for its photo-catalytic properties and enhanced corrosion resistance in aqueous environments. Due to these properties TiO2 is very attractive material for light-induced self-cleaning glass, water-cleaning and producing hydrogen from water applications. Numerous works are dedicated to the diffusion of various dopants like niobium or chromium in TiO2 but so far, none studied the self-diffusion of titanium in nanocrystalline TiO2. The grain boundary self-diffusion in thin nanocrystalline TiO2 films is investigated. The oxide films are produced using a novel deposition method from metal-organic precursors at relatively low (400-500°C) temperatures. A relaxation annealing at 800°C was performed. The diffusion was measured in temperature interval between 200°C and 600°C by means of the radiotracer technique applying the 44Ti isotope and utilizing ion beam sputtering for sectioning. The diffusion was measured at different oxygen pressures. In addition, the microstructure and its possible evaluation during diffusion annealing was investigated using TEM. The results are discussed with respect of the relationship between grain boundary self-diffusion and the synthesis pathway, the oxygen pressure and resulting microstructure of the nanoscale functional oxide films.

MM 20: HV Mrovec

Time: Wednesday 10:15–10:45 Location: IFW A

Invited Talk MM 20.1 Wed 10:15 IFW A

Atomic-scale modeling of dislocations in iron — •Matous Mrovec — Fraunhofer IWM, Freiburg, Germany — IZBS, Karlsruhe Institute of Technology, Karlsruhe, Germany

Mobilities of screw and edge (or mixed) dislocations in α-iron, like in other bcc metals, are markedly different at low temperatures. While the mobility of edge dislocations remains large and independent of temperature, the mobility of screw dislocations decreases strongly with decreasing temperature. The reason of this distinct behavior has been traced to a non-planar core structure of the 1/2<111> screw dislocation. The non-planar core is primarily responsible for most peculiarities in mechanical behavior of α-iron and other bcc metals such as the strong temperature dependence of the flow and yield stresses, the brittle-to-ductile transition, and the non-Schmid behavior.

We performed extensive atomistic simulations of dislocation properties in α-Fe using a recently constructed magnetic bond-order potential. This potential is based on the tight binding theory of chemical bonds and is therefore able to capture non-saturated covalent di-

rectional bonds originating from the d-electrons as well as magnetic interactions. It is also computationally efficient so that it enables to simulate complex dislocation configurations under arbitrary stress conditions. We will discuss the behavior of dislocations at the atomic scale and show how the atomistic studies enable to formulate mobility laws that can be implemented in mesoscopic discrete dislocation dynamics studies of large dislocation ensembles.

MM 21: Topical Session Electron Theory I

Time: Wednesday 11:00–13:00 Location: IFW A

Topical Talk MM 21.1 Wed 11:00 IFW A

Materials design based on ab initio thermodynamics: Development of accurate and efficient multiscale strategies — •Jörg Neugebauer, Blazej Grabowski, Fritz Körmann, Martin Friak, and Tilmann Hickel — Max-Planck-Institut für Eisenforschung, Düsseldorf

The combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts has quickly advanced in the past few years and allows now to tackle even complex engineering systems such as polycrystals or steels. Key to these studies is the highly accurate determination of free energies and surfaces. In the first part of the talk it will be shown how efficient sampling strategies together with high convergence density-functional theory calculations allow an accurate determination of all relevant temperature dependent free energy contributions such as electronic, harmonic, anharmonic, magnetic and structural excitations. Using these results to construct coarse grained models stability issues and mechanical properties of various alloys have been computed. The flexibility and the predictive power of this approach will be discussed in the second part of the talk for a few examples: Martensitic transitions in magnetic shape memory alloys, the design of novel light weight alloys, failure mechanisms in novel steels and unraveling design principles in biological structural materials.

Topical Talk MM 21.2 Wed 11:30 IFW A

Diffuse scattering methods as a testbed for alloy theory — •Harald Reichert — European Synchrotron Radiation Facility, 38043 Grenoble, France

Based on high energy x-ray scattering we have developed new experimental tools in order to reveal details in the energetics of binary alloys with very high accuracy. The technique allows to collect scattering patterns in planes or, more recently, in 3D volumes in reciprocal space. High energy X-ray scattering is characterized by a large Ewald sphere. Similar to transmission electron microscopy, it is possible to map entire planes in reciprocal space with a single exposure employing 2D detectors. In the time-resolved mode the technique allows to follow phase transformations in-situ. In parallel, we have combined first-principles calculations of the alloy energetics with reciprocal space methods for the interpretation of the experimentally determined diffuse scattering maps. This has allowed us to separate chemical and strain-induced components in the effective pair interactions and visualize competing interactions in binary alloys. Applications of this general scheme to a number of binary metallic alloy systems will presented.

Topical Talk MM 21.3 Wed 12:00 IFW A

From electronic structure to real materials properties: Concepts and realization — •Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

Due to their predictive power, methods based on electronic structure theory are more and more applied for modelling real materials properties within a quantum mechanical framework. From a technical point of view, the vision behind is the design of functional materials with special properties before expensive experiments are performed. For this, the combination of different methods is a must to describe materials' behaviour from the atom up to the microstructure. In this contribution, recent developments, possibilities and limitations to study real materials properties by first-principles methods will be discussed. It will be shown that the application of an atomistic approach to materials allows for the quantitative description of properties, e.g. ordering parameters and phase boundaries, defects and dislocation behaviour, compressibility and elastic constants or piezo-response tensors and dielectric constants. Regarding systems, the examples reach from metal alloys and adsorption systems to niobates and hybrid materials.

MM 21.4 Wed 12:30 IFW A

Atomistic modelling of interfaces between cubic phases and topologically close-packed phases in refractory metals — •Thomas Hammerschmidt[1], Bernhard Seiser[2], Miroslav Cak[1], Ralf Drautz[1], and David G. Pettifor[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]MML, University of Oxford, United Kingdom

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the mechanical properties and is attributed to high local concentrations of refractory elements. It is well known that the structural stability of these phases is driven by the average d-band filling. We demonstrate that this structural trend can be understood with a canonical d-band tight-binding model by comparing to our extensive density-functional theory calculations for tcp phases. In order to understand the precipitation of tcp phases, we investigate the structure and energetics of interfaces between the cubic phases bcc and fcc and the topologically close-packed phases σ and A15. In particular, we employ analytic bond-order potentials (BOPs) that provide an approximation to the tight-binding model and are suitable for large-scale atomistic simulations. We demonstrate the applicability of recently parametrised BOPs for refractory elements to the description of tcp phases at elevated temperatures and report on the first dynamic simulations of interfaces between cubic phases and topologically close-packed phases.

MM 21.5 Wed 12:45 IFW A

Tight-binding simulation of complex metallic alloys — •Eunan J. McEniry, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

The interplay between various co-existing phases of metallic alloys is a key factor in the determination of the strength, ductile and magnetic properties of modern steels. While ab-initio density-functional theory provides an accurate description of the electronic and mechanical properties of metallic systems, the methodology is prohibitively expensive when applied to larger multi-component systems. While empirical interatomic potentials can be applied to such systems, there are significant question marks over the transferability of these models when applied to systems to which they have not been fitted. The tight-binding approach lies in an intermediate region, enabling the simulation of several thousands of atoms, while retaining the essential physics of bonding and cohesion in solids,

The aim of the present work is to produce a systematic approach which is generally applicable to the full block of transition metals, and which can be applied directly within existing scale-bridging methodologies. We have therefore developed a general tight-binding approach for the simulation of complex metallic alloys, in which the parameterisation is obtained directly from ab-initio calculations. In order to assess the quality and transferability of the approach, we have extensively applied the resulting models to a wide range of alloy structures.

MM 22: Topical Session TEM VI

Time: Wednesday 11:00–13:00 Location: IFW B

Topical Talk MM 22.1 Wed 11:00 IFW B

In-situ TEM: Atomistic Insights into Crystallisation — •Christina Scheu — Department of Chemistry & Center for NanoScience (CeNS), Ludwig-Maximilians-University, Munich, Germany

Ultrathin non-conducting nanowires are potential candidates for application in electronic devices and for medical treatments. Recently we studied the self-catalytic vapor-liquid-solid (VLS) growth of alumina nanowires in-situ at 750 degrees Celsius in a high voltage transmission electron microscope [1]. The atomic scale observation revealed that the growth of the nanowire in [0001] direction takes place layer-by-layer involving a two-step mechanism. Oscillatory growth and dissolution reactions alternate at the top rim of the nanowire which is in contact to the liquid Al droplet and the vapor phase leading to periodical changes of the triple junction configuration. The dissolution reaction of the crystalline top rim supplies the oxygen which is required to grow a new (0006) alumina layer [1]. The growth of the (0006) layer is relatively fast since the Al atoms in the liquid adjacent to the crystalline alumina wire possess already similar position as in the solid [2]. This leads to an easy pathway for the interfacial diffusion of oxygen. The rate limiting step for growth of the alumina nanowire is the oxygen transport after completion of a new (0006) alumina layer when the crystalline rim is formed.

[1] Oh, Chisholm, Kauffmann, Kaplan, Luo, Rühle, Scheu, Science 330, 489 (2010). [2] Oh, Kauffmann, Scheu, Kaplan, Rühle, Science 310, 661 (2005).

Topical Talk MM 22.2 Wed 11:30 IFW B

Quantitative Nanoscale Analysis in 3D using Electron Tomography — •Christian Kübel — Karlsruhe Institute of Technology, INT, 76344 Eggenstein-Leopoldshafen, Germany

State-of-the-art electron tomography has been established as a powerful tool to image complex structures with nanometer resolution in 3D. Especially STEM tomography is used extensively in materials science in such diverse areas as catalysis, semiconductor materials, and polymer composites mainly providing qualitative information on morphology, shape and distribution of materials. However, for an increasing number of studies quantitative information, e.g. surface area, fractal dimensions, particle distribution or porosity are needed. A quantitative analysis is typically performed after segmenting the tomographic data, which is one of the main sources of error for the quantification. In addition to noise, systematic errors due to the missing wedge and due to artifacts from the reconstruction algorithm itself are responsible for these segmentation errors and improved algorithms are needed.

This presentation will provide an overview of the possibilities and limitations of quantitative nanoscale analysis by electron tomography. Using catalysts and nano composites as applications examples, intensities and intensity variations observed for the 3D volume reconstructed by WBP and SIRT will be quantitatively compared to alternative reconstruction algorithms; implications for quantification of electron (or x-ray) tomographic data will be discussed and illustrated for quantification of particle size distributions, particle correlations, surface area, and fractal dimensions in 3D.

MM 22.3 Wed 12:00 IFW B

In-situ Transmission Electron Microscopy of Material Transport and Crystallization during the Al induced layer exchange (ALILE) process — •Balaji Birajdar[1], Tobias Antesberger[2], Martin Stutzmann[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Materials Science Department VII, University of Erlangen-Nürnberg, Germany — [2]Walter Schottky Institut and Physics Department, Technische Universität München, Germany

The ALILE process enables fabrication of thin polycrystalline Si films at relatively low temperatures, making it highly promising for applications in thin film photovoltaics. While the driving forces for the metal-induced crystallization are rather well understood, the details of the material transport during the layer exchange are largely unknown. In this work, the microstructure of a stack of a-Si(100nm)/Al(50nm)/quartz, annealed at 450°C, has been investigated at different length scales by combining optical microscopy, SEM, and TEM. The results indicate that the layer exchange and crystallization proceeds by forming 20-50 μm wide dendritic cells with Al deficient centers. Excessive upward transport of Al by epitaxial growth out of the existing Al grains into the a-Si was observed in a rim of about 10 μm width around these cells and, to a smaller extent even beyond. Using in-situ TEM, the lateral and vertical transport of Al at the expanding crystallization front could be directly visualized for the first time and is proposed to be caused by Coble-type diffusion of Al driven by the compressive stress in the Al layer.

MM 22.4 Wed 12:15 IFW B

In situ tensile testing of Au nanowires — •Burkhard Roos[1], Bahne Kapelle[1], Gunther Richter[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Max-Planck-Institut für Metallforschung, 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 size-dependent 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. In wires with diameters above 180 nm, full dislocation based deformation and dislocation storage is observed. Wires with diameters below 180 nm show a different deformation behaviour. Stacking faults appear during deformation as a result of the nucleation and motion of partial dislocations. The stacking faults form homogenously along the wire length and appear and disappear in less than 50 ms. The stacking faults do not move as the wire is further deformed, but may eventually thicken into nanotwins through the sequential activation of partial dislocations on neighbouring (111) planes. Post-deformation TEM studies show that fracture often occurs at a nanotwin. A possible explanation for the dependence of the deformation mode on wire diameter and stress will be discussed in terms of the splitting distance of partial dislocations.

MM 22.5 Wed 12:30 IFW B

Optimization of STEM Tomography Acquisition - A Comparison of Convergent Beam and Parallel Beam STEM Tomography — •Johannes Biskupek, Jens Leschner, Paul Walther, and Ute Kaiser — Central Facility of Electron Microscopy, Ulm University, Ulm, Germany

In this work two imaging modes available in state-of-the-art scanning transmission electron microscopes (STEM) are compared: conventional STEM with a convergent beam (nanoprobe) and STEM with a parallel beam (microprobe). The effect and influence of both modes with respect to their depth of field are investigated using standard gold cross grating TEM samples. It will be shown that microprobe posses a large depth of field (up to +/-30 micron), thus, all features are kept in focus even at high tilt without the necessity to apply specimen topology-dependent dynamic focus. A decrease of measured FWHM of gold beads at high tilt by a factor of three shows a gain in resolution by microprobe STEM and the advantage over conventional nanoprobe STEM imaging. Test tomograms are acquired, aligned, reconstructed, and evaluated using both modes. It is shown that STEM using the microprobe mode produces tomograms with fewer distortions and artifacts and allows resolving finer features. Microprobe STEM tomography is advantageous when semi thin TEM samples (ca. 500 nm thick) are imaged at relatively low magnification with a large field of view (more than 3 by 3 micron).

We acknowledge the DFG for financial support within the collaborative research centre SFB 569 and the project KA 1295-7/1.

MM 22.6 Wed 12:45 IFW B

3D electron tomography of biological photonic crystals — •Benjamin Butz[1], Benjamin Winter[1], Benito Vieweg[1], Isabel Knoke[1], Stefanie Spallek[1], Gerd Schröder-Turk[2], Klaus Mecke[2], and Erdmann Spiecker[1] — [1]CENEM, Universität Erlangen-Nürnberg — [2]Theoretische Physik I, Universität Erlangen-Nürnberg

Photonic crystals, i.e. periodical nanostructures of materials with different dielectric constants, are highly interesting for applications in optics, optoelectronics, and sensing. By tailoring the geometrical pa-

rameters radically different and improved optical properties (e.g., optical band-gap structure, extreme refractive indices, or high anisotropy) can be achieved. Naturally occurring photonic crystals, like butterfly scales, exoskeletons of insects (chitin), or seashells (nacre), can serve as model systems for understanding the relationship between structure and optical properties. Butterfly scales are studied by TEM using a FEI Titan^3 80-300 instrument. An optimized FIB technique or ultramicrotome sectioning were used to prepare the sensitive specimens with desired thickness. Since the periodical structures have dimensions on the sub-μm scale, HAADF-STEM tomography was employed for obtaining extended tilt series under conditions of atomic-number sensitive imaging. Since the solid crystal consists of chemically homogeneous chitin while the pores are unfilled, the distinct contrast in the images can easily be interpreted in terms of the local projected mass density allowing to reconstruct the chitin distribution within the optical unit cell of the scales with high 3D resolution.

MM 23: Phase Transformations I

Time: Wednesday 11:00–13:15 Location: IFW D

MM 23.1 Wed 11:00 IFW D

Junction controlled grain growth: evolution equations and grain size distributions — •Peter Streitenberger and Dana Zöllner — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

Normal grain growth is essentially controlled by the grain boundaries. However, the other structural elements of a 3D grain network (triple lines and quadruple points) may have likewise a strong effect on the growth kinetics but at very small grain sizes. For a systematic estimation of the influence of the energetic and kinematic properties of boundary junctions on grain growth each type of junction is assigned an own specific energy and mobility. By application of a thermodynamic variation principle a general grain evolution equation is derived.

Apart from the already known size parameters associated with finite boundary junction mobilities two further size parameters associated with non-vanishing specific energies of triple lines and quadruple points enter the calculation. Consequently, apart from linear and exponential kinetics already considered by Gottstein, Shvindlerman and others, six further types of growth kinetics can be identified at very small grain sizes. Each type of growth kinetics is characterised by a separable scaling form of the grain evolution equation from which analytical expressions of the corresponding self-similar size distribution function are derived. The obtained size distributions of triple and quadruple junction limited grain growth are clearly shifted to smaller relative sizes indicating a strong population enhancement in this range.

MM 23.2 Wed 11:15 IFW D

In-situ Messungen von magnetisch getriebener Korngrenzenbewegung in Zink-Bikristallen — •Christoph Günster — RWTH Aachen, Aachen, Deutschland

In der vorliegenden Arbeit wurde die magnetisch getriebene Korngrenzenbewegung in hochreinen (99.995%) Zink-Bikristallen untersucht. Die Beweglichkeit von <10-10>-Kippkorngrenzen mit Desorientierungswinkeln zwischen 60° und 90° wurden bestimmt. Aufgrund der magnetischen Anisotropie von Zink, können unter dem Einfluß eines externen Magnetfeldes Korngrenzen (KGen) von einer magnetischen treibenden Kraft angetrieben werden. Die Ergebnisse bestätigen, daß eine ausgeprägte Abhängigkeit der KGen-Beweglichkeit zur Desorientierung besteht. Darüber hinaus besaßen die gemessenen Bewegungsaktivierungsparameter für ebene, asymmetrische KGen deutlich höhere Werte, als dies in der Vergangenheit für krümmungsgetriebenen KGen in Zink-Bikristallen berichtet wurde. Nach weiteren Experimenten an symmetrischen KGen wurden deutlich niedrigere Aktivierungsparameter festgestellt als bei unseren Experimenten an asymmetrischen KGen, was einen Hinweis auf die Existenz einer ausgeprägten Inklinationsabhängigkeit der Beweglichkeit von Kipp-KGen in Zink darstellt. Weiterhin unterstützen diese Daten unsere Ergebnisse aus früheren Experimenten an symmetrischen und asymmetrischen Kipp-KGen mit Bi-Bikristallen. Weiterhin sind diese Ergebnisse ein Hinweis auf das Ablaufen jeweils unterschiedlicher atomistischer Mechanismen bei der Bewegung von symmetrischen und asymmetrischen Kipp-KGen in Zink.

MM 23.3 Wed 11:30 IFW D

In situ three-dimensional investigation of Ostwald ripening — •Thomas Werz[1], Uwe Wolfram[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, University of Ulm, Germany — [2]Institute of Orthopaedic Research and Biomechanics, University Hospital Ulm, Germany

Owing to their destructive nature, conventional techniques for investigating Ostwald ripening — the thermally induced coarsening of two-phase microstructures — do not allow repeated observation of the same volumetric region in a sample. In this work, we employed laboratory microcomputed tomography (microCT) to carry out nondestructive, three-dimensional characterization of an Al-5 wt.% Cu alloy undergoing Ostwald ripening. The sample was repeatedly annealed at 630°C, inducing a semisolid state with a volume fraction $V_V = 60\%$ of the coarsening (solid) phase. Each annealing step was followed by a microCT scan performed at room temperature. When semisolid, the system consists of Al-rich grains surrounded by a liquid phase of higher Cu content. Tomographic contrast between the two phases arises from their differing attenuation factors for x-ray radiation. During cooling, the liquid phase tends to retreat into the triple junctions, resulting in incomplete coverage of the boundaries separating the coarsening grains. Correction for the latter effect was accomplished by a watershed-transform-based image processing routine, enabling reliable grain segmentation and the evaluation of local and global microstructural parameters in 3D. These can, in turn, be compared to theoretical and simulation results.

MM 23.4 Wed 11:45 IFW D

Microstructural investigation and thermal stability of ball-milled Fe-Cu — •Catharina G. Wille and Tala'at Al-Kassab — King Abdullah University of Science and Technology (KAUST), Materials Science and Engineering, Thuwal 23955-6900, Kingdom of Saudi Arabia

The microstructural changes upon heat treatment in ball-milled Fe-10at.%Cu powders after different milling times from 2 to 10h were observed by means of transmission electron microscopy (TEM). This heat treatment was performed isochronally inside a differential scanning calorimeter (DSC).

The heat release calculated from the DSC curves will be correlated to the observed microstructural changes. Additionally the positions of the exothermic peaks and the respective stored enthalpies will be compared to the ones obtained within earlier works and especially their conclusions on phase separation - accompanied by grain growth and strain release.

For the minority component copper as well as for the impurity oxygen the segregation and precipitation behaviour in connection with grain growth were investigated by atom probe tomography (APT).

MM 23.5 Wed 12:00 IFW D

Advanced Characterization of High Performance Permanent Magnets for Hybrid Electric Vehicles — •Thomas George Woodcock and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, PO Box 270116, 01171 Dresden, Germany

NdFeB sintered magnets have recently found important new applications in electric motors for hybrid electric vehicles (HEV) and in the generators used in wind turbines. The operating temperature of the electric motor in HEV is typically approx. 180°C and therefore magnet grades with high Dy content are required in order to provide a sufficiently large coercivity at such temperatures. The limited availability of Dy has led to a very high and somewhat fluctuating price of that element. Significant research effort has therefore recently been put into reducing the Dy content or eliminating the need for Dy in NdFeB sintered magnets for high temperature applications. In addition to various experimental routes toward achieving this, novel approaches yielding detailed microstructural characterisation are required in order to bring greater understanding of coercivity mechanisms. High resolution SEM and TEM, magneto-optical Kerr microscopy and MFM are routinely used to examine a range of NdFeB materials. Recent developments include the use of aberration-corrected TEM to obtain highest

spatial resolution images and the application of electron backscatter diffraction (EBSD) to obtain crystallographic orientation data on a local scale from all the phases present in the microstructure. The combination of EBSD and EDX with high resolution serial sectioning yields 3D orientation and chemical data which will also be discussed.

MM 23.6 Wed 12:15 IFW D

Surface studies of Fe polycrystals with LEEM — •Benjamin Borkenhagen[1], Thorsten Franz[2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]ELMITEC GmbH, Albrecht-von-Grodeck-Str. 3, 38678 Clausthal-Zellerfeld

Low energy electron microscopy (LEEM) has been proven a versalite tool for studies on single crystal surfaces. In this contribution, we present the application of LEEM to study the microstructure and processes on surfaces of polycrystals. The additional capability of this microscope to acquire low energy electron diffraction patterns of crystallites (μ-LEED) allowed us to distinguish between different crystallographic surface structures. We observed atomically flat terraces separated by monoatomic steps as well as facetted surfaces. Islands with regular shapes were detected at the surfaces of some crystallites. In situ investigations during heating of the polycrystal showed that these islands were bulk impurities which segregated to the surface, or diffused back to the bulk depending on temperature. Parallel imaging of the whole field by LEEM enabled the observation of dynamic processes such as grain boundary motion and segregation processes at elevated temperatures.

MM 23.7 Wed 12:30 IFW D

Ground state structure in Au-50 at.% Pd — •Cédric Sax[1], Bernd Schönfeld[1], and Andrei Ruban[2] — [1]LMPT, Department of Materials, ETH Zurich — [2]KTH Stockholm, Sweden

From experiment no ordered structure is known for the bulk Au-Pd system. Electronic structure calculations indicate the CH structure for 1:1 stoichiometry, diffuse scattering also allows plausible candidates for ordered structures to be discussed. In this work diffuse x-ray scattering was measured at room temperature from a single crystal of Au-48 at.% Pd. The crystal was aged at 703 K to set up a state of thermal equilibrium. The short-range order scattering is characterized by $2k_F$ maxima where k_F is the Fermi wave vector along <110>. From the separated short-range order scattering effective pair interaction parameters were determined. Ordering energies were calculated for several $L1_0$-based long-period superstructures (LPS) as LPS are favorably formed in systems with $2k_F$ maxima. These results from diffuse scattering will be compared with those from recent electronic structure calculations.

MM 23.8 Wed 12:45 IFW D

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

We investigate the kinetics of crystal growth by measurements of the dendrite growth velocity as a function of undercooling during non-equilibrium solidification. Measurements are conducted under different conditions of convection. The liquid samples are levitated and undercooled in strong alternating electromagnetic fields leading to forced convection. Inductive stirring is avoided by processing the samples in a glassy slag where only natural convection is present. Forced convection and natural convection can be reduced by performing undercooling experiments in reduced gravity. The experimental results obtained under different conditions are compared to each other in order to investigate the influence of convection on the growth dynamics of dendrites in undercooled melts. The congruently melting compound Ni_2B is chosen as a suitable sample system. It forms an intermetallic phase with growth velocities that are comparable to the fluid flow velocities in electromagnetically levitated melts. The results are analyzed within dendrite growth models and reveal that the growth velocity is essentially influenced by forced convection in strong electromagnetic fields. The present work is supported by DFG under contract HE1601/25.

MM 23.9 Wed 13:00 IFW D

Phase Formation and Martensitic Transformation of Cast Cu-Zr-Co Alloys — •Fatemeh A. Javid[1], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [2]Technical Uneversity, Dresden, Germany

The phase formation and martensitic transformation of $Cu_{50-x}Zr_{50}Co_x$ ($x = 0, 2, 5, 7.5, 10, 20$ at.%) melt-spun and suction-cast bulk specimens has been studied. X-ray analysis shows that cobalt affects the eutectoid reaction $CuZr \leftrightarrow Cu_{10}Zr_7 + CuZr_2$ of the binary Cu-Zr system and shifts it to lower temperatures. The results indicate that in compositions with at least 5 at. % cobalt, the glass crystallizes directly into B2(Cu,Co)Zr and this phase is the equilibrium phase at room temperature. An extended solid solution $Cu_{50-x}Zr_{50}Co_x$, cobalt between 5 and 50 at.% is indicated by the lattice parameter of the B2-type phase versus Co-content. The X-ray analysis of bulk specimens shows that in compositions with more that 10 at. % of cobalt, the B2(Cu,Co)Zr phase is coming from the liquid directly and this is the main phase at room temperature while compositions with less that 10 at.% of cobalt contain monoclinic CuZr phases as the main phase. Martensitic transformation of bulk samples was investigated with differential scanning calorimeter and the results show that cobalt shifts the transformation temperatures to lower temperatures. The martensite transformation start temperature lowers from about 452 K for $x = 0$ to room temperature for $x = 7.5$.

MM 24: HV Finnis

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

Invited Talk MM 24.1 Wed 14:00 IFW A

Statistical thermodynamics of defects and interfaces in metals — •Michael W. Finnis — Department of Materials and Department of Physics, Imperial College London, Exhibition Road, London SW7 2AZ

In order to make more impact in metal physics, and especially engineering, theorists working at the atomic scale are turning increasing attention to understanding and predicting high temperature properties. One of the challenges this entails is the application of statistical mechanical techniques, via computer simulation, using models based on electron theory for calculating internal energies. In this talk I will briefly review how techniques for free energy calculation (classical density functional theory, atomistic thermodynamics, biased molecular dynamics sampling, such as metadynamics and Wang-Landau methods) are being linked to techniques for internal energy calculation, with examples of our work including point defect concentrations, melting temperature and solid-liquid interfacial free energies in general. The emphasis is on how we can go beyond regular solution theory and the quasi-harmonic approximation. 1. Hagen, M. et al, Point defects and chemical potentials in ordered alloys. Phil. Mag. A 1998, 77, 447-464. 2. Angioletti-Uberti, S. et al, Solid-Liquid Interface Free Energy through Metadynamics Simulations. Phys. Rev. B 2010, 81, 125416.

MM 25: Topical Session Electron Theory II

Time: Wednesday 14:30–15:30 Location: IFW A

Topical Talk MM 25.1 Wed 14:30 IFW A

The LDA+DMFT approach to the electron theory of strongly correlated metals — •Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg

A better understanding of the physics of realistic strongly correlated electron systems in the metallic state is one of the key ingredients in order to describe a wide range of novel solid state compounds. The complex competition between the localized and the itinerant character of interacting electrons in a manifestly multi-orbital scenario within a given (anisotropic) crystal structure is giving rise to highly interesting phenomena, such as, e.g., intricate magnetic behavior. By combining the dynamical mean-field theory (DMFT) with the local-density approximation (LDA) to density functional theory, a powerful many-body technique is established to tackle the given problem on a truly realistic level. Here the basics and the current status of the LDA+DMFT method as well as its possible future in the context of generic first-principles approaches beyond the realm of conventional exchange-correlation functionals will be discussed. On a technical level, the emphasis will be on the currently relevant interfacing steps between the Kohn-Sham band picture and the DMFT many-body representation. Results of selected materials studies will provide an insight into the high capability of the outlined framework.

MM 25.2 Wed 15:00 IFW A

Transferable tight binding description of the Fe-C interaction — •Nicholas Hatcher, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

A coherent transferable tight-binding (TB) parameterization of charge transfer and electronic potentials has yet to be developed for the Fe-C interaction. Additionally, while interatomic potentials have been obtained for this interaction, recent findings show that the results from these potentials are inconsistent with DFT calculations and do not give an accurate portrayal of chemical bonding in the system. Using dual DFT grid and LCAO calculations within GPAW, we obtain one electron wave functions expanded in a multiple-ζ LCAO basis. This is down-folded onto a optimal minimal basis, giving a continuous and transferable description of Fe-C bonding. By constructing a TB energy functional using these bond integrals and a parameterized interatomic repulsion, we show how an accurate description of the energy hierarchy of relevant Fe-C structures, including the interstitial occupancy of carbon in iron, can be achieved. This simple model based on physical insights may be used to study systems containing thousands of atoms.

MM 25.3 Wed 15:15 IFW A

Charge transfer and localization within a tight binding framework — •Georg K. H. Madsen, Eunan J. McEniry, Nick Hatcher, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

The computational cost of density functional theory (DFT) places limitations on its application to both extended defects and to sampling the configuration space of complex phases. While these problems can be treated by empirical potentials, these can be questioned both from a view of transferability and physical justification.

From a computational point of view and from the wish to gain physical insight, one successful intermediate method between DFT and empirical potentials is the tight-binding (TB) method. In its conventional form the TB method models the total energy as a repulsive pair potential and a bonding many-body term. Using a down-folding technique we demonstrate how TB parameterizations can be constructed which involve a minimum number of fitting parameters and are based as closely as possible on the DFT energy functional.

We will discuss transition metal oxides and long range charge transfer within a tight binding framework based on the second order expansion of the DFT energy functional.

MM 26: Topical Session TEM VII

Time: Wednesday 14:30–15:30 Location: IFW B

Topical Talk MM 26.1 Wed 14:30 IFW B

Electron Holography for structures and fields at a nanoscale — •Hannes Lichte[1], Dorin Geiger[1], Andreas Lenk[1], Martin Linck[1,2], Axel Lubk[1,3], Falk Roeder[1], John Sandino[1,4], Jan Sickmann[1], Karin Vogel[1], and Daniel Wolf[1] — [1]Triebenberg Laboratory, Institute for Structure Physics, TU Dresden, 01062 Dresden, Germany — [2]National Center for Electron Microscopy Lawrence Berkeley National Laboratory One Cyclotron Road, MS 72-150 Berkeley, CA 94720 — [3]CEMES-CNRS - Groupe NanoMatériaux 29, rue Jeanne Marvig B.P. 94347 F-31055 Toulouse Cedex — [4]Facultad de ciencias Universidad Nacional de Colombia Sede Bogota, Colombia

TEM is the method of choice for analysis of materials at atomic scale at point resolution below 0.1nm allowing interpretation of positions of atoms e.g. at interfaces. However, the phases are lost, and hence the electric and magnetic fields in the object. Phase-loss is overcome by electron holography [1]. This allows access to **Inner Potentials in solids **Functional potentials such as pn-junctions **Electric fields controlling growth in biominerals **Depolarizing fields in ferroelectrics **Magnetic fields in magnetic structures **difference of atomic numbers **number of atoms in an atomic column **Coherence of inelastically scattered electrons Lateral resolution of 0.1nm is reached. Phase resolution presently is about 2p/70, just at the edge for detecting interatomic electric fields. [1] H. Lichte, M. Lehmann, Rep. Prog. Phys. 71 (2008), 016102. Funding by DFG,German-Israel Funds (GIF), European Union (Framework 6 Integr. Infrastruct., Reference 026019 ESTEEM).

MM 26.2 Wed 15:00 IFW B

Strain mapping of strained transistors by dark-field off-axis electron holography — •Jan Sickmann[1], Hannes Lichte[1], Holm Geisler[2], and Hans-Jürgen Engelmann[2] — [1]Triebenberg Laboratory, Institute for Structure Physics, TU Dresden, 01062 Dresden, Germany — [2]Globalfoundries Dresden, Center for Complex Analysis, 01109 Dresden, Germany

Dark-field off-axis electron holography in a TEM has been proven to measure the two-dimensional strain distribution in semiconductor devices at nanometer scale resolution [1]. The technique is based on the interference of diffracted waves from adjacent sample areas using the dark-field off-axis holography configuration [2]. The phases of the diffracted waves then give direct access to local changes in the lattice parameter [1]. We present recent results of strain measurements on state-of-the-art transistor structures manufactured by Globalfoundries Dresden. Applying specific holographic setups at an aberration corrected Tecnai F20 TEM lead to significant improvements in lateral resolution and signal resolution of the two dimensional strain maps. Since the variations of the lattice strain relative to the original lattice parameter are often expected to be less than 1%, possibilities for optmizing the signal properties are discussed. [1] M. J. Hÿtch, F. Houdellier, F. Hüe, and E. Snoeck, Nature London 453, 1086 (2008). [2] K.-J. Hanszen, J. Phys. D: Appl. Phys 19, 373 (1986).

MM 26.3 Wed 15:15 IFW B

Untersuchung struktureller und optischer Eigenschaften von getemperten InGaNAs-Trögen mittels TEM-Dreistrahl-Abbildung — •Robert Imlau[1], Knut Müller[1], Marco Schowalter[1], Bernardette Kunert[2], Rafael Fritz[2], Kerstin Volz[2], Wolfgang Stolz[2] und Andreas Rosenauer[1] — [1]Universität Bremen, D-28359 Bremen — [2]Universität Marburg, D-35032 Marburg

In diesem Beitrag werden strukturelle und optische Eigenschaften von $In_{0.2}GaN_{0.024}As$-Quantentrögen vor und nach einer Temperaturbehandlung unter N_2 Atmosphäre bei 600°C untersucht und verglichen. Die Messung von Stickstoff- und Indiumkonzentration basiert auf der Auswertung von Verzerrung und chemisch sensitivem Kon-

trast in einer TEM-3-Strahlabbildung der Reflexe 000, 200 und 220. Alle Bilder wurden an einem Cs-korrigierten Titan 80/300 aufgenommen. Proben homogener Dicke wurden mittels FIB und Niederenergie-Ionenmühle präpariert. Absorptionsmessungen zeigen eine Blauverschiebung der Bandlücke von 38 ± 7 meV nach dem Tempern. Da die mittels 3-Strahlabbildung erhaltenen In- und N-Konzentrationsprofile keine langreichweitige Umverteilung beider Elemente zeigen, wird die beobachtete Blauverschiebung u.a. im Hinblick auf bevorzugte In-N Koordination nach der Temperung diskutiert.

MM 27: Phase Transformations II

Time: Wednesday 14:30–15:45 Location: IFW D

MM 27.1 Wed 14:30 IFW D

In-situ characterization of embedded metallic nano-clusters with a positron beam. — •Philip Pikart[1,2] and Christoph Hugenschmidt[1,2] — [1]ZWE FRM-II, Garching, Germany — [2]Technische Universität München, Physikdepartment E21, Garching, Germany

Positron measurements on model systems of aluminum with thin embedded layers (0.5nm to 100nm) of different materials (Au, Cr and Cu) are reported. It is shown how the positron affinity of different metals affects the measurements sensitivity. It is demonstrated that temperature dependent Doppler broadening on gold clusters embedded in aluminum reveals clustering and re-organization processes.

When a positron is implanted into a sample, it thermalizes rapidly (within ps) and starts to diffuse over up to several hundred lattice constants. During the diffusion it can be trapped at irregularities in the crystal matrix. Hence it acts as a "nanoprobe" with a highly increased sensitivity e.g. for vacancy-like defects and metallic agglomerations. The non-destructiveness of this method enables in-situ observation of agglomeration growth at different temperatures. The usage of a mononergetic positron beam assures the positron implantation into the bulk where surface effects do not influence the measurement.

MM 27.2 Wed 14:45 IFW D

Morphological study of a peritectic Al-Ni alloy by a quantitative phase-field simulation — •Julia Kundin and Heike Emmerich — 1Material and Process Simulation (MPS), University Bayreuth, Germany, Nürnberger str.38(4) 95448 Bayreuth

A phase field model of simulating peritectic and eutectic growth is described, which is applied to the investigation of the peritectic microstructure in an Al-Ni alloy during directional solidification. The presented model is an extension of the multiphase-field approach [I. Steinbach, Physica D 94 (1996), R. Folch and M. Plapp, Phys. Rev. E 72, 011602 (2005)] to study the solidification of multiphase systems based on the real free energy functions. It is shown, that the model is a reliable and powerful numerical approach to simulate the solidification of alloys involving more than one solid phase at nonisothermal conditions. The model is verified on an example of the Al-Ni system for which the morphology of the peritectic structure during the process of the directional solidification is investigated. The proposed model is also extended to multi-component systems.

MM 27.3 Wed 15:00 IFW D

Phase-field simulation of dendritic growth in the system Al-Si — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Materials and Processes, Karlsruhe, Germany

The strength of the phase-field method to simulate material alloy systems has been demonstrated over the years. The method however, requires the knowledge of the Gibbs-free energy of the phases involved in the transition which can be derived via the Calphad method. In the present study, we build the methodology for the direct use of thermodynamic databases in the simulation of material alloys, using the phase-field method. Using this set-up, we investigate the effect of small additions of a third component on dendritic growth in the cast Al-Si system. In particular, we study the effect of these additions on the dendritic arm spacing, in a directional solidification setup and attempt to derive relationships between the amount of additions of the third component and the physical parameters like interfacial surface tensions, through systematic parameter studies and comparison with experiments.

MM 27.4 Wed 15:15 IFW D

Recrystallization of a deformed 3D microstructure studied by macro-micro simulations — •Alexander Vondrous[1], Michael Selzer[1], Britta Nestler[1], Pierre Bienger[2], and Simone Schendel[3] — [1]Institute of Materials and Processes, University of Applied Sciences, Karlsruhe, Germany — [2]Fraunhofer Institut for Machanics, Freiburg, Germany — [3]Institute for Reliability of Components and Systems KIT, Karlsruhe, Germany

Cold rolling of sheet metal introduces a high amount of dislocations, which lead to significant changes of the material properties. During annealing, to obtain the initial properties, dislocations are reduced by nucleation and growth of the nuclei driven by the stored energy (recrystallization). A dislocation density triggered nucleation of recrystallizing grains is introduced to simulate stored energy driven nuclei growth of cold rolled sheet metal for static recrystallization. The phase-field model incorporating additional equations for the stored energy driving force is introduced. Growth kinematics depend on the crystallographic orientations and the stored energy distribution. The starting point of the microstructure simulation is a macroscopic finite element simulation containing the corresponding deformation texture and accumulated plastic slip. A comparison with experimental measurements is achieved by evaluating the pole figures of the polycrystalline material at different stages of the process. The comparison serves as a validation of the micro-macro approach.

MM 27.5 Wed 15:30 IFW D

On the Growth Behaviour of Individual Grains in Polycrystals — •Dana Zöllner[1], Peter Streitenberger[1], and Iain Fielden[2] — [1]Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, UK

A 3D grain growth model is developed allowing the prediction of the growth history of individual grains. The model - based on a generalised mean-field approach - represents data of 3D grain growth - simulated by a Monte Carlo Potts model algorithm - very well. The parameters from the obtained grain size distribution are then used to calculate an analytic function describing the individual growth history of all grains. A comparison with simulation results of normal grain growth shows good agreements for the temporal development of grain sizes of single grains as well as for the prediction of their life span.

On the other hand, the monitoring of the motion of individual quadruple points and triple junctions in 2D sections of the simulated 3D microstructures shows a highly discontinuous movement. Based on a stochastic grain growth model the diffusivity of the Brownian-like motion can be related to the average growth rate providing a possibility to determine the average growth law of the grain ensemble solely from the stochastic growth behaviour of single grain features.

In addition, the simulation results - compared with real-time in-situ SEM observations of grain growth - show a good qualitative agreement of the temporal movement of grain boundary junctions.

MM 28: Topical Session Electron Theory III

Time: Wednesday 15:45–17:15 Location: IFW A

MM 28.1 Wed 15:45 IFW A

Parameterization of bond-order potentials from first principles — Martin Reese[1,2], •Matous Mrovec[2,1], Christian Elsässer[2,1], Alexander Urban[3], and Bernd Meyer[3] — [1]IZBS, Karlsruhe Institut of Technology, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany — [3]ICMM and CCC, University of Erlangen-Nürnberg, Erlangen, Germany

Bond-order potentials (BOPs) provide a real-space semi-empirical description of interactions between atoms based on the chemically intuitive tight-binding approximation for the electronic structure. The BOP approach offers two key advantages that are crucial for a successful modeling of extended crystal defects in covalent materials and transition metals. First, due to its quantum mechanical character it conveys a physically sound description of chemical bonding rather than ad hoc functional forms, which are common to classical empirical interatomic potentials. Second, its real space parameterization and computationally linear scaling enables to carry out computer simulations of large and complex systems, which are usually inaccessible to rigorous first-principles density-functional-theory (DFT) methods. We will present a recently developed atomic-orbital-projection approach that enables to construct BOPs for transition metals and their compounds in a rigorous manner from DFT results via tight-binding models. The success of these BOPs will be demonstrated on studies of extended defects, in particular lattice dislocations and grain boundaries.

MM 28.2 Wed 16:00 IFW A

Bond-Order Potentials for bcc Transition Metals Niobium and Tungsten — •Miroslav Cak, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universitat Bochum

Bond-order potentials (BOPs) are derived from the tight-binding approximation by expanding the density of states in local moments contributions. The BOPs provide comparable accuracy as tight-binding at less computational cost and a better scaling behavior. While the previously developed BOPs involve numerical evaluation of the response (Green's) function, the expressions for the bond energy and related interatomic forces are analytical within the formalism of the analytic BOPs. In this contribution, we present the parametrisation of analytic BOPs for the bcc transition metals Niobium and Tungsten. The parameters were optimised for the equilibrium bcc structure and extensively tested for atomic environments far from equilibrium that have not been considered in the fitting procedure. These tests include structural energy differences for competing structures; tetragonal, trigonal, hexagonal and orthorhombic deformation paths; formation energies of point defects and phonon dispersion relations. Comparison of these calculations with corresponding calculations using density-functional theory and numerical BOPs demonstrates a very good transferability of our analytic BOPs to atomic structures of experimentally relevant complexity.

Topical Talk MM 28.3 Wed 16:15 IFW A

Hydrogen in metals, atomic defects in crystals, and wetting phenomena. - The benefit of using density functional theory — •Lothar Schimmele — Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Examples from three different research areas will be discussed in order to demonstrate how ab-initio electron theory can contribute to a quantitative understanding of complex physical behaviour of materials if it is used in combination with theoretical models, statistical mechanics, and experiment.

For a proper description of hydrogen in solids quantum effects on the nuclear motion have to be included in the modelling. Some methods and simple results are presented.

In order to quantify, e.g., concentrations of atomic defects a statistical theory of defect equilibria is required.

Finally some ideas as to a systematic route from ab-initio investigations to a mesoscopic and macroscopic description of capillarity are presented.

MM 28.4 Wed 16:45 IFW A

First-principles simulations of H interstitials within Σ3 and Σ5 grain boundaries in bcc Fe — •Yaojun Du, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität, Bochum, Germany

Hydrogen impurities in steels can degrade the mechanical properties of the host material. Due to the complex nature of hydrogen-embrittlement (HE), the underlying HE mechanism has not been fully understood. One possible cause is that H impurities may weaken the bonding of Fe atoms near the grain boundaries, leading to an embrittlement of the bulk material. In this work, we study the interaction of H interstitials with Σ3 and Σ5 grain boundaries (GBs) in bcc Fe, and investigate the migration processes of H within the GBs, using density functional theory. Our results indicate that the GBs that we studied provide energy traps of 0.4-0.5 eV for H interstitials, and these trapped H interstitials may facilitate the crack growth at the GB interface. For the Σ5 bcc Fe GB we find that the fast diffusing H within Fe bulk region can be readily trapped to the GB interface with an escape barrier of 0.6 eV. On the other hand, the trapped H interstitial can perform a relatively slow migration within the interface with a diffusion barrier of 0.25 eV. We are now carefully computing the transition rates among inequivalent H sites within the Σ5 bcc Fe GB. These results will serve as input for a lattice kinetic Monte Carlo model to study the dynamics of H diffusion in the vicinity of the GB.

MM 28.5 Wed 17:00 IFW A

Effect of H on homogeneous dislocation nucleation: Consequences for hydrogen embrittlement — •Johann von Pezold and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The embrittlement of modern high-strength steels is commonly explained by the HELP (Hydrogen-Enhanced Local Plasticity) mechanism. In its original form this mechanism attributes the embrittlement to a localized increase in plasticity resulting from a hydrogen-induced shielding of the stress fields of pre-existing dislocations. Recent in situ electrochemical nano-indentation experiments [1] suggest that H also reduces the critical shear stress for the homogeneous nucleation of dislocations in a range of metals. The observed reduction in the critical shear stress was correlated to a H-induced decrease in the stacking fault energy and/or shear modulus of the host material, as well as an increased dislocation core radius. In this study the model is evaluated using density-functional theory. In particular, the effect of H on the shear modulus and the stacking fault energy in Al, Ni and Cu was determined. Preliminary results indicate a significant reduction in the shear modulus and a moderate reduction in the stacking fault energy with increasing H content, in line with the originally proposed model. Whether or not the observed reduction in the critical shear stress for the dislocation nucleation can be explained by this model will depend on the H solubility under the elevated H chemical potential conditions in the in situ nano-indentation experiments.

[1] A. Barnoush and H. Vehoff, Acta. Mat. 58, 5274 (2010).

MM 29: Topical Session TEM VIII

Time: Wednesday 15:45–17:00 Location: IFW B

MM 29.1 Wed 15:45 IFW B

Quantitative TEM-EDX analysis of compositional inhomogeneities in CIGS absorbers — •Isabel Knoke[1], Benito Vieweg[1], Stefan Jost[2], Jörg Palm[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nuürnberg, Cauerstraße 6, 91058 Erlangen — [2]AVANCIS GmbH & Co. KG, Otto-Hahn Ring 6, 81739 München

Thin film solar cells based on the chalcopyrite absorber material $Cu(In,Ga)(S,Se)_2$ are promising candidates for reducing the costs of photovoltaic [1]. However, depending on the fabrication process the absorber may show strong compositional inhomogeneities resulting in local variations of the band gap. Since these inhomogeneities occur on

various length scales and both, in horizontal and vertical layer direction, characterization by TEM techniques is difficult because of missing depth information and limited thin area in conventional plan-view and cross-section samples, respectively. A new sample preparation technique overcomes these limitations by a double-wedge geometry that separates depth information in a continuous series of thin slices that are spread over a lateral distance [2]. Application of this preparation technique allows us to perform a significant number of EDX measurements at the same layer height and determine variations in the In/Ga resp. S/Se ratios. Corresponding changes in the lattice constant and band gap are calculated.

[1] J. Palm, V. Probst, F.H. Karg, Solar Energy 77, 757 (2004) [2] E. Spiecker et al., Acta Mater. 55, 3521 (2007)

MM 29.2 Wed 16:00 IFW B

Determination of Nitrogen Concentration in Dilute GaNAs by STEM HAADF Z-Contrast Imaging — •Tim Grieb[1], Knut Müller[1], Oleg Rubel[2], Rafael Fritz[2], Marco Schowalter[1], Kerstin Volz[2], and Andreas Rosenauer[1] — [1]Universität Bremen, D-28359 Bremen — [2]Universität Marburg, D-35032 Marburg

Incorporation of small amounts of nitrogen into III-V semiconductors such as GaAs reduces their band gaps which makes these alloys interesting for diverse applications. As only low N-concentrations are needed, composition analyses require highly sensitive methods. In this contribution we show that high-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) allows accurate determination of composition in diluted GaNAs, based on comparison of experimental with simulated reference images. HAADF intensity is affected by atomic number (Z-contrast), thermal-diffuse scattering (TDS), and Huang scattering at static atomic displacements (SADs). For GaNAs, conventional simulations based on frozen lattice multislice algorithms that include TDS let expect a lower HAADF-STEM contrast compared to pure GaAs, but experimental results show a contrary ratio. The observed contrast can be obtained by taking SADs into account that are caused by the comparatively small covalent radius of N atoms. The SADs are computed by relaxation of super cells via valence force field calculations and implemented into the STEMsim simulation software. Considering SADs we present quantitative evaluation of concentration in $GaN_{x<0.05}As_{1-x}$ quantum wells that agree with strain state analysis and X-ray diffraction measurements.

MM 29.3 Wed 16:15 IFW B

Quantitative local profile analysis of nanomaterials based on TEM diffraction — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

A method yielding a quantitative profile analysis from selected area electron diffraction patterns (PASAD, www.univie.ac.at/pasad) has been worked out. The results gained by PASAD can be combined with the local information from TEM images to study various nanomaterials. It can be used for the analysis of inhomogeneous materials, ultrathin nanocrystalline films, nanoparticles and nanosized ordered domains. As an example the grain size reduction by thermal annealing in nanocrystalline FeAl is shown in the present study. Nanocrystalline FeAl was made by severe plastic deformation resulting in the loss of the long-range order. Thermal annealing leads to the recurrence of the B2 superstructure, the recovery of dislocations, the sharpening of grain boundaries and an unexpected reduction in grain size. To study these processes, both the coherently scattering domain (CSD) size and the grain size were monitored during annealing by TEM methods. The CSD size was determined using PASAD and the grain size was determined from analysing dark field images: the CSD size increases by a factor of 2 while the grain size is reduced by a factor of 2. It is concluded that the decrease of the grain size during annealing is caused by the re-arrangement of dislocations forming new boundaries, that is linked to the recurrence of the long-range order.

MM 29.4 Wed 16:30 IFW B

Diffraction spots off the diffraction rings in severely deformed bulk nanocrystalline FeAl — •Anna Findeisen, Christoph Gammer, Christian Rentenberger, and Hans-Peter Karnthaler — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

The bulk intermetallic compound FeAl (processed with high purity Fe and Al) is made nanocrystalline by severe plastic deformation (SPD) applying the method of repeated cold rolling and folding. For the transmission electron microscopy (TEM) study thin foils were prepared by ion milling. TEM shows in the nanocrystalline structure grain sizes $<$100 nm. As expected the electron diffraction patterns show diffraction rings due to the different orientation of the nanograins. In addition to the diffraction spots lying on the rings, several spots are encountered that lie clearly off the rings. The TEM study reveals that these additional spots are not arising by an epitaxial oxide or other components. The analysis leads to the clear result that these spots are caused by moiré effects since their diffraction vectors can be constructed by adding the vectors of appropriate spots on the rings. Moiré effects are expected to occur in TEM of bulk nanocrystalline materials when the grain size is small and especially when the density of subgrainboundaries is high. The latter is confirmed by the fact that the occurrence of additional spots is more pronounced in the present case than in materials made nanocrystalline by other SPD methods. It also agrees with the results of differential scanning calorimetry showing in the present study higher values of enthalpies connected with the different peaks.

MM 29.5 Wed 16:45 IFW B

TEM Studies on Etch Pit Formation during the Nucleation of 3C-SiC on Si(001) — •Julian Müller[1], Philip Hens[2], Peter Wellmann[2], and Erdmann Spiecker[1] — [1]CENEM, University Erlangen-Nuremberg — [2]I-MEET, University Erlangen-Nuremberg

Due to its interesting electronic properties, cubic silicon carbide (3C-SiC) is widely investigated by many research groups. However, appropriate methods for bulk crystal growth are still lacking making it necessary to fabricate 3C-SiC in an epitaxial growth process. In view of microelectronic applications Si(001) is the most interesting substrate for epitaxial growth of 3C-SiC but the enormous lattice misfit (ca. 20%) leads to a high density of microstructural defects like dislocations, stacking faults and micro twins.

Within this work different heating rates have been applied during the growth of an initial 3C-SiC nucleation layer on Si(001) to investigate the impact on the final layer quality. It turned out that fewer grains nucleate at faster heating rates resulting in an improved layer quality. By TEM a new type of etch pit was detected, which differs from the well-known faceted voids reported in the literature. TEM investigations unambiguously revealed that the etch pits are filled with a continuous film of highly defective SiC. Both, the voids and the etch pits penetrate into the silicon. The etch pit formation can be ascribed to the contamination of the epitaxial deposition system with residual carbon, for which reason the cleanliness of the reaction chamber is proposed to be a crucial parameter for the growth of epitaxial 3C-SiC.

MM 30: Complex Materials

Time: Wednesday 16:15–17:15 Location: IFW D

MM 30.1 Wed 16:15 IFW D

Numerical solutions of the elastodynamic equations for icosahedral quasicrystals — •Frohmut Rösch and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The vibrational properties of most solids can be characterized by the time evolution of the phononic displacements $\mathbf{u}(\mathbf{x}, t)$. In quasicrystals, however, additional degrees of freedom must be taken into account, which are described by the so-called phasonic displacements $\mathbf{w}(\mathbf{x}, t)$. The latter are related to flips of atoms in the atomic picture.

The governing equations, which describe the dynamic behavior of both $\mathbf{u}$ and $\mathbf{w}$, are extensions of the elastodynamic equations for crystals generalized by the phasonic degrees of freedom. These result in propagating (phonon-like) and diffusive (phason-like) elementary modes.

A finite element package has been adjusted to solve the elastodynamic equations for a three-dimensional icosahedral quasicrystal. Fundamental scenarios, e.g. the time evolution of phason and phonon excitations in a finite sample, are investigated and compared to analytic

solutions.

MM 30.2 Wed 16:30 IFW D

Effective potentials for phonon dynamics in clathrates — •Daniel Schopf and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

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 interaction of the phonons with local vibration modes ("rattling") of these guest atoms inside the host framework.

For computational studies of dynamic properties long simulation times and large samples are required. This makes first principle calculations of these structures, even with very fast computers, very unfeasible. Classical molecular dynamics, however, can easily handle large systems and long simulation times. The potentials needed for these MD simulations can be obtained from ab-initio calculations with the force-matching method. It uses large numbers of reference data to fit an effective potential that can reproduce the forces, energies and stresses of the ab-initio calculation.

To model the strongly directional atomic interactions in clathrates, angular dependent potentials are required. An analytic potential will be presented to model these systems. The phonon dynamics of clathrates was studied with these potentials and will be compared with ab initio results.

MM 30.3 Wed 16:45 IFW D

Eigenstates and electronic transport in the generalized Labyrinth tiling — •Stefanie Thiem and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Understanding the physical properties of quasicrystals requires a deeper insight into the nature of the eigenstates of these systems and their relation to the transport properties. We present results for d-dimensional quasiperiodic models based on the metallic mean sequences constructed by the inflation rule $\mathcal{P}_a = \{x \to y, y \to yxy^{a-1}\}$, where x and y denote the strengths of the two bond types. The eigenstates of the quasiperiodic chain are obtained by numerical diagonalization of the tight-binding Hamiltonian. Higher dimensional solutions of the associated generalized labyrinth tiling are constructed then by a product approach from the one-dimensional eigenstates, allowing the numerical consideration of large systems up to 10^{11} sites. Thereby, we obtain information about the localization of the wave functions by investigating the scaling behavior of the participation ratio and about the electronic properties by studying the scaling behavior of the wave packet spreading with time. We present results for different scaling exponents and investigate their relations in order to obtain a better understanding of the characteristics of quasicrystals.

MM 30.4 Wed 17:00 IFW D

Order Parameter Dynamics in the quasi two-dimensional Charge Density Wave System $2H-TaSe_2$ — •Tim Huber[1], Hanjo Schäfer[1], Helmuth Berger[2], and Jure Demsar[1] — [1]Physics Department, Universität Konstanz,78457, Germany — [2]Institut de Physique de la Matiere Complexe, EPFL, 1015 Lausanne, Switzerland

Recent results of time-resolved spectroscopy on the quasi one-dimensional charge density wave (CDW) system $K_{0.3}MoO_3$ have shown that on a short timescale, the electronic and lattice parts of the CDW order parameter are disentangled (Schäfer et al., PRL 105, 066402 (2010)). Here we present the data on the quasi two-dimensional CDW system $2H-TaSe_2$ and show - utilizing a time-dependent Ginzburg-Landau model - that they can be interpreted within the same theoretical framework. We demonstrate that also in the quasi two-dimensional case, the appearance of low frequency Raman active modes and their T-dependence can be naturally explained by linear coupling of the electronic part of the order parameter to the $2k_f$ phonons. Compared to $K_{0.3}MoO_3$, however, in $2H-TaSe_2$ the electronic part of the order parameter faster follows the lattice, demonstrated by stronger mode softening as T_c is approached. In addition, we present the first study on Cu-intercalated $2H-TaSe_2$ which shows a dramatic increase in the CDW transition temperature compared to its parent compound.

MM 31: Postersitzung II

Time: Wednesday 17:15–18:45 Location: P5

MM 31.1 Wed 17:15 P5

Structure-optimization of the Ξ-phases in the Al-Pd-Mn system — •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

The Ξ-phases – with ξ and ξ' being the simplest ones – are probably the most investigated ternary phases. The experimental structure refinement of ξ' carried out by Boudard et al. dates back more than 10 years. Almost all present studies rely on this structure proposal. Here we present an optimization of the Boudard model using a combination of classical molecular dynamics and density functional theory. We determine an optimal configuration for the Al atoms on the innermost shell of the pseudo-Mackay clusters (PMC). These Al atoms could not be resolved very accurately in experiment. Furthermore, we examine the "glue" atoms, i.e. those not belonging to any PMC. In order to get an estimate for the stability of a phase the ground state energies are calculated relative to other binary and ternary compounds coexisting in the Al-Pd-Mn system. The results are applied to the ξ_1'-phase (ε_{16}) where the projections of the PMC columns form pentagons and nonagons.

MM 31.2 Wed 17:15 P5

Refined model of phason flips in quasicrystals using kinetic Monte Carlo simulations — •Hansjörg Lipp and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

HRTEM observations of decagonal Quasicrystals by Edagawa et al. [1] show that phason flips can be observed directly as spots which vanish or appear erratically. The spots can be interpreted as clusters of atoms, which move coherently. Compared to the time scale of atomic jumps (picoseconds), this process is surprisingly slow, flips occur in periods of seconds or even minutes.

We study this phenomenon using several statistical model systems, e.g. based on a structure model for d-Al-Cu-Co suggested by Zeger et al. [2], where rings of ten atoms can perform flips by collective motion of atoms inside decagonal double layers. Using kinetic Monte Carlo simulations [3], we investigate how flip frequencies depend on the number of decagonal layers and on the variations of the local energy landscape.

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

MM 31.3 Wed 17:15 P5

Structural changes of Gd thin films and islands during hydrogen absorption — •Sara Wanjelik, Georg Oeltzschner, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

We report on the effects of hydrogen absorption in Gadolinium Systems by using scanning tunneling microscopy (STM) and spectroscopy (STS).

Offering low amounts of hydrogen (1-2 L) to thin films results in the adsorption on the surface. Adsorbed hydrogen changes the electronic structure of the affected areas due to supression of the surface state of Gd (0001). After the subsequent diffusion of hydrogen into the underlying layer the surface state reappears. This can be observed using STS and STM. This change in the electronic structure causes a voltage dependent corrugation which changes sign at 0.8 V. It was observed that the inversion of the corrugation for islands occurs at higher voltages.

For higher dosage (>50 L) not only the electronic structure is affected but also the topographic structure. As a result we found small circular islands (diameter 6-8 nm) and ramp-like structures exhibiting the height of one atomic step. The topographic change of the surface

can be ascribed to hydride formation (GdH_2) in the thin film. This obsevation will be compared to the behavior of islands during hydrogen absorption.

MM 31.4 Wed 17:15 P5

Electrochemical analysis of SiNWs anodes in lithium-ion batteries according to the amount of copper deposition — •Gibaek Lee[1,2], Gaelle Offranc-Piret[3], Fracois Ozanam[3], Stefan L. Schweizer[2], and Ralf B. Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials Halle — [2]Martin-Luther-University Halle-Wittenberg — [3]Ecole Polytechnique, France

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 alloying/de-alloying, resulting in mechanical disintegration of electrode and rapid capacity fading. Addition of inactive but conductive elements into silicon can improve electrical connection of particles and suppress volume change.

In this study, we prepared oriented silicon nanowires (SiNWs) array on n-type silicon substrate by electroless etching in aqueous HF solution containing $AgNO_3$, and then filled in SiNWs, with copper by electrodeposition in aqueous solution. The material characteristics and anodic performance of copper deposited SiNWs anodes have been examined.

MM 31.5 Wed 17:15 P5

Band engineering for thermoelectric materials — •Mingxing Chen and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

Engineering of the electronic band structure of Ge-based skutterudites and clathrates is of importance for optimizing their thermoelectric properties in terms of Seebeck coefficients. Alloys of $FM_4Sb_xGe_{12-x}$ skutterudites and $Ba_8M_xGe_{46-x}$ clathrates (F: filler atom, M: metal) are investigated by means of density functional theory calculations from which the transport properties are derived by Boltzmann transport theory within the constant relaxation time approach[1]. For a large Seebeck coefficient it is important to place the Fermi energy close to a gap. Therefore, we analyse the nature of gap formation for these two classes of materials and derive a simple counting rule for chemical optimization of the thermoelectric properties [2]. Following this rule, our data on skutterudites reveal that partially replacing Ge by Sb leads to the desired placement of the Fermi energy. For clathrates, also the electric resistivities are analyzed which reveal characteristic temperature dependent features in agreement with experiment[2].

[1] G. K. Madsen and D. J. Singh, Comput. Mater. Sci. 175, 67 (2006). [2] I. Zeiringer, Mingxing Chen et al., submitted.

MM 31.6 Wed 17:15 P5

Epitaxy, lift-off and surface treatment of Ni-Mn-Ga based magnetic shape memory alloy films — •Marcus Müller and S. G. Mayr — Leibniz-Institut für Oberflächenmodifizierung, Translationszentrum für regenerative Medizin und Fakultät für Physik und Geowissenschaften der Universität Leipzig, 04318 Leipzig

During the past years much progress has been achieved in the field of magnetic shape memory alloys. The Ni-Mn-Ga alloy is presumably the most prominent representative, which can yield strains as high as 10% in highly tailored single crystals. Freestanding miniaturized single crystalline films on the other hand are much less explored and face several challenges, particularly including single crystalline growth and film lift-off. Using magnetron sputtering from Ni-Mn-Ga compound target we fabricate single-crystalline-like epitaxial Ni-Mn-Ga films on a heated MgO (100) substrate, which transform to the martensite phase upon cooling down to room temperature [1]. A recently-developed etching technique [2] for direct removal of the MgO substrate is subsequently employed for lifting these films off the substrate, which is currently being optimized further. As a main advantage the present approach does not require buffer layers, which would possibly prove harmful at the elevated temperatures employed for epitaxy. With the aim of enhancing biocompatibility, coating concepts are furthermore explored.

[1] G. Mahnke, M. Seibt, S.G. Mayr, Phys. Rev. B 78, 012101 (2008)

[2] T. Edler, S.G. Mayr, Adv. Mat. (in press, 2010)

This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909.

MM 31.7 Wed 17:15 P5

Proton conductivity of imidazole molecules encapsulated in imogolite nanotubes. — •Barbara Supronowicz, Agnieszka Kuc, and Thomas Heine — SES, Jacobs University Bremen, Bremen, Germany

Proton conduction in solids has gained a lot of attention because of promising variety of applications, such as proton exchange membranes (PEMs) and fuel cells.[1a] The choice of PEM has an influence on the efficiency of fuel cell. Due to stability and electronic properties[2] imogolite has been chosen as a host structure for proton carriers. The presence of water molecules has a significant influence on the proton conductivity[3]. To avoid the dependence of proton conductivity on the temperature, different proton carrier * imidazole * was introduced into the structure instead of water molecules.[1]

All the structures were investigated using SCC- DFTB method.[4]

[1] a) Kreuer, K.D. Chem. Mater. 1996, 8, 610-641. b) Goward, G.R., et al. J. Phys. Chem.B.,2002, 106, 9322-9334.

[2] Guimaraes, L.; Enyashin, A.N.; Frenzel, J., et al. ACS NANO, 2007,1, 362-368.

[3] Cukierman, S.; Biochimica et biophysica acta- bioenergetics, 2006, 1757, 876-885.

[4] Elstner, M; Porezag, D. et al. Phys. Rev. B.,1998, 58, 7260-7268.

MM 31.8 Wed 17:15 P5

Evaluation of perovskite oxides as oxygen evolving catalyst for photocatalytic water splitting — •Daniel Mierwaldt[1], Jörg Hoffmann[1], Bruno Jasper[1], Christian Jooss[1], Stephanie Raabe[1], Sven Schnittger[1], and Simone Techert[2] — [1]Institut für Materialphysik, Universität Göttingen — [2]MPI für biophysikalische Chemie, Göttingen

In search for suitable water splitting catalysts, several oxide materials have already been successfully investigated. However, most of them have band gaps in the UV-region limiting the efficiency in light harvesting. Perovskite manganites represent a promising material class, in which strong electron-lattice coupling results in a broad polaronic absorption band from visible light to near-IR. In addition, multilevel excitation into long-living polaronic states may contribute to high chemical potentials of electron-hole pairs, exceeding the band gap of the respective material.

In this contribution the strongly correlated $CaMnO_3$ has been investigated, which reveales a rather large exchange current density of about 1,9 mA/cm^2. Bulk samples as well as epitaxial grown thin films on Nb-doped $SrTiO_3$ substrate were investigated by means of cyclic voltammetry. The samples were used as working anode in a photocatalytic apparatus with Pt-counter cathode in Na_2SO_4-electrolyte.

A complementary approach to water splitting is the use of nano composites forming two dimensional patterns of pn-junctions. First results on the photocatalytic activity of Nb-doped $SrTiO_3$ (n-type) mixed with off-stoichiometric $CoFe_2O_4$ (p-type) are presented.

MM 31.9 Wed 17:15 P5

Niobium doped SrTiO3 and p-type CoFe2O4 nanocomposite films for photoelectric applications — •Bruno Jasper, Daniel Mierwaldt, Andreas Blumenstein, Sven Schnittger, Jörg Hoffmann, and Christian Jooss — Institute of Material Physics, University of Göttingen, Germany

Patterned arrays of pn-junctions are interesting model systems for the study of photocatalytic and photovoltaic applications. In this field, self-organizing systems show promising results with respect to simple preparation and increasing efficiency. As an example of self-organized oxide structures we present a study of nanocomposites composed of strontium titanate (SrTiO3) and cobalt ferrite (CoFe2O4) prepared by reactive ion beam sputtering. Doped SrTiO3 is a photoactive material allowing water splitting. Properly doped CoFe2O4 is a good conductor which serves well as a catalyst in hydrogen production. Voltage-cyclometric measurements reveal photo-catalytic activity of single phase Nb:SrTiO3 as well as the SrTiO3-CoFe2O4 nanocomposite films. Furthermore, first results on the fabrication of n-type niobium doped strontium titanate (Nb:SrTiO3) and off stoichiometric p-doped cobalt ferrite (p:CoFe2O4) by self-organized decomposition are presented. The structural and chemical properties of the samples are examined by scanning electron microscopy, X-ray diffraction, transmission electron microscopy and energy dispersive X-ray spectroscopy.

MM 31.10 Wed 17:15 P5

Material Test Facilities for Solar Absorber of Solar Tower Power Plants — Bernhard Hoffschmidt, Konstantin Kon-

stantin Geimer, Oliver Kaufhold, and •Markus Sauerborn — Solar-Institut Jülich (SIJ), FH Aachen, Heinrich-Mußmann-Str. 5, D-52428 Jülich

Since 2009 the first and only German solar tower power plant the large scale test facility Solar Tower Juelich is in operation. The SIJ has initiated the construction phase and is now with the German Aerospace Center/DLR exclusive involved in the accompanying research. The central receiver plant features as central innovation an open volumetric receiver, consisting of porous ceramic elements that simultaneously absorb the concentrated sunlight and transfer the heat to ambient air passing through the pores so that an average temperature of 680°C is reached. The subsequent steam cycle generates up to 1.5MWe. To analyze the capability of new absorber specimen under realistic conditions or optimize the structures several special labor test facilities had been developed at the SIJ. An interesting one is using a powerful near-infrared radiator to simulate concentrated solar light. It offers a beam power of up to 300W/m* for test samples with a surface of about 14x14cm and the absorber surface can reach more than 1000°C. To suck ambient air through the open absorber - like on the tower - it is mounted on a special compressor system. An easy and quick change of the absorber specimen makes it possible to test new absorber structures fast and reproducible under various radiation conditions. An overview about the test facility and some results of the last years will be given.

MM 31.11 Wed 17:15 P5

SIMS study on the surface elemental distribution in AISI type 304 steel — •Chika Izawa[1], Stefan Wagner[1], Vladimir Burlaka[1], Mauro Martin[2], Sebastian Weber[2], Anais Bourgeon[3], Richard Pargeter[3], Thorsten Michler[4], and Astrid Pundt[1] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin / Ruhr-Universität Bochum, Universitätsstr. 150 - IA 2/44, D-44801 Bochum — [3]TWI Ltd, Granta Park, Great Abington, Cambridge CB21 6AL, United Kingdom — [4]Adam Opel GmbH, IPC R2-50, GM Alternative Propulsion Center Europe 65423 Ruesselsheim

Hydrogen embrittlement of low-Ni austenitic stainless steels is suggested to occur due to strain-induced surface alpha -martensite, since the hydrogen diffusivity in bcc phases is expected to be much higher than in the austenitic phase. But, also the local surface chemistry might be responsible for the steel susceptibility. The surface chemistry on two different surface conditions of AISI 304 was investigated by Secondary Ion Mass Spectrometry: a. directly after the machining process and b. after solution annealing process. For both AISI 304 surfaces a layered stacking of Fe- and Cr-oxide was found. The oxide layer thickness was about 5 nm for sample a., and about 10 nm for sample b. The chemical mapping on sample a. shows relatively homogeneous elemental distributions due to the fine microstructure of martensite. For sample b, Fe, Ni, SiO2, FeO and NiO are segregated at the grain boundaries. In contrast, Cr and CrO are distributed in grains.

MM 31.12 Wed 17:15 P5

Gezielte Strukturmodifizierung der MOFs zur Optimierung von Sorptionseigenschaften — •Olga Khvostikova[1,2], Lars Giebeler[1], Bassem Assfour[3], Gotthard Seifert[3], Helmut Hermann[1] und Helmut Ehrenberg[1] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 27 01 16, D-01171 Dresden, Germany — [2]Institut für Werkstoffwissenschaft, TU Dresden, Helmholtzstr. 7, D-01069 Dresden, Germany — [3]Institut für Physikalische Chemie, TU Dresden, Bergstr. 66b, D-01062 Dresden, Germany

MOFs sind eine relativ neue Verbindungsklasse in der Festkörperchemie, wobei die Abkürzung MOF für Metal-Organic Framework, metallorganische Gerüststruktur, steht.

Wasserstoffspeicherung in diesen hochporösen Materialien wird als eine vielversprechende Strategie für die Entwicklung der on -board Technologie bei Kraftfahrzeugen betrachtet.

Die Herstellung von Materialien mit kleinen Poren, das Dotieren mit hydrogenophilen Metallen, ein anderes Konnektorkation oder die Variation von Brückenliganden sind mögliche Wege zur Optimierung der Materialien und der Erzeugung von effektiven Wasserstoffspeichern.

Im Rahmen der Forschungsarbeit werden MOF - Materialien zur Bestimmung der Einflüsse von unterschiedlichen Strukturparametern und Präparationsverfahren auf die Wasserstoffspeicherkapazität gezielt hergestellt und auf ihre Wasserstoffspeichereigenschaften untersucht.

MM 31.13 Wed 17:15 P5

Hydrothermal synthesis and physical properties of LiXPO4 (X = Mn, Fe, Co, Ni or mixtures) — •Carsten Jähne[1,2], Christine Täschner[2], Bernd Büchner[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, 69120 Heidelberg — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden

Due to their high open circuit voltages (OCV), materials with phosphor olivine structure are of great interest for application as positive-electrodes in secondary batteries. However, the low electrical conductivity of olivine materials results in a low power capability which demands downscaling of the crystallites in order to enhance surface to volume ratio and/or appropriate post-treatment techniques. Here we report on low temperature conventional and microwave-assisted hydrothermal synthesis of LiXPO4 (X = Mn, Fe, Co, Ni or mixtures of these). In particular, we present electron microscopy, x-ray diffraction and magnetization data on the resulting material which allow to determine the phase, the morphology and the valence of the transition metal ions.

MM 31.14 Wed 17:15 P5

Deuterium trapping in graphite and carbon films growing under irradiation by deuterium plasma — •Vladimir Burlaka[1,2], Yuriy Gasparyan[2], Aleksandr Pisarev[2], Aleksandr Rusinov[2], Stepan Krat[2], and K. Sugiyama[3] — [1]University of Goettingen, Germany — [2]National Research Nuclear University "MEPhI", Moscow, Russia — [3]Max-Planck-Institut für Plasmaphysik, Garching, Germany

Carbon is planned to be used in the divertor of ITER until the tritium phase. Its further use is under discussion for possible high tritium inventory. In the case of graphite or other carbon-based materials, essentially four mechanisms have been identified for the uptake and retention of hydrogen: buildup of a saturated surface layer, chemisorption on inner porosity surface, intergranular diffusion and trapping, and co-deposition of hydrogen with carbon on plasma-exposed surfaces. This work was motivated by the investigation of hydrogen trapping in graphite and co-depositing carbon films growing by the plasma irradiation. A new laboratory plasma device for investigation of plasma surface interaction was constructed. Ion pickup research, surface modification, re-deposition of the sputtered material and combined carbon and hydrogen deposition from the plasma, were performed. Used analysis techniques: thermal desorption spectroscopy (TDS), SEM, AFM and Nuclear reaction analyses (NRA).

MM 31.15 Wed 17:15 P5

SIMS study on the surface elemental distribution in AISI type 304 steel — •Chika Izawa[1], Stefan Wagner[1], Vladimir Burlaka[1], Mauro Martin[2], Sebastian Weber[2], Anais Bourgeon[3], Richard Pargeter[3], Thorsten Michler[4], and Astrid Pundt[1] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin / Ruhr-Universität Bochum, Universitätsstr. 150 - IA 2/44, D-44801 Bochum — [3]TWI Ltd, Granta Park, Great Abington, Cambridge CB21 6AL, United Kingdom — [4]Adam Opel GmbH, IPC R2-50, GM Alternative Propulsion Center Europe 65423 Ruesselsheim

Hydrogen embrittlement of 8 wt-% Ni, 18 wt-% Cr austenitic stainless steels is suggested to occur due to strain-induced surface $\alpha-$martensite, since the hydrogen diffusivity in bcc phases is expected to be much higher than in the austenitic phase. But, also the local surface chemistry might be responsible for the steel susceptibility. The surface chemistry on two different surface conditions of AISI 304 was investigated by Secondary Ion Mass Spectrometry(SIMS): a. directly after the machining process and b. after solution annealing process. The chemical mapping on sample a. shows relatively homogeneous elemental distributions due to the fine microstructure of martensite. For sample b, larger grains are observed. At the grain boundaries, Fe, Ni, SiO_2, FeO and NiO are segregated. In contrast, Cr and CrO are distributed in grains. Financial support from the Bundesministerium für Wirtschaft und Technologie (BMWi), 0327802C is gratefully acknowledged.

MM 31.16 Wed 17:15 P5

Intercalation Mechanism and Aging Effects in LiFePO4 as Cathode Material for Li-Ion-Cells — •Birte Riechers, Sebastian Mathes, Carsten Nowak, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

Since Lithium Iron Phosphate was recently established as a cathode material for high-current Li-Ion cells, intercalation mechanisms and aging effects in this material come to the forefront of scientific investigations. An enhanced understanding of time- and cycling-mode dependent changes of Li-intercalation processes of LiFePO4 contributes to these efforts. Using commercial, self-prepared, and thin-film model Li-ion cells, microstructural changes and aging effects are investigated using (in-situ) SEM, XRD.

The progress of degradation depending on electrolyte, method of cell preparation, and cycling conditions is studied. The homogeneous intercalation structure of pristine cells changes to a spatially heterogeneous structure due to different intercalation kinetics and phase distributions. This occurs even within single cathode material particles. Thin-film model cell cathode intercalation processes are being compared to the behaviour of cathodes consisting of particles.

MM 31.17 Wed 17:15 P5

Investigation of the heterogeneous nucleation in the peritectic AlNi alloys — •Julia Kundin[1], Hai-Lin Chen[2], Heike Emmerich[1], and Rainer Schmid-Fetzer[2] — [1]Material and Process Simulation (MPS), University Bayreuth, Germany, Nürnberger str.38(4) 95448 Bayreuth — [2]TU Clausthal, Inst. Metallurgie, Robert-Koch-Str. 42 38678 Clausthal-Zellerfeld Germany

A quantitative multi-phase field model is used for the simulation of the solidification and for stages of peritectic transformation in the binary Al-Ni alloy. The experimental DSC curves were used for the calibration of the model and the evaluation of the kinetic parameters and the nucleation rate. For the simulation of the heat flow the temperature correction method have been employed. The model can be employed to obtain new relations between processing parameters and resulting kinetics and dynamics of the phase-transformation processes. The model and the method of the calibration could be applicable to any alloy systems with the known thermodynamic data.

MM 31.18 Wed 17:15 P5

Exploring the interface structure of TaN/Gd_2O_5/HfO_2 gate stacks — •Catharina G. Wille, Dongkyu Cha, J. Alfonso Caraveo, Husam N. Alshareef, and Tala'at Al-Kassab — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

The recent introduction of high dielectric constant (high-k) oxides such as HfO_2 as replacement materials for the SiO_2 gate dielectric has accelerated research activity in high-k materials for transistor-based devices.

In this study, a Gd_2O_5/HfO_2 stacked gate dielectric was used to fabricate TaN/ Gd_2O_5/HfO_2 /SiO_2/Si thin films and MOS capacitors. The effects of annealing condition on the structure and morphological properties of the proposed films were investigated via transmission electron microscopy (TEM). As shown in earlier works, DFT calculations in conjunction with the electrical and physical characterization of the gate stacks demonstrated the importance of controlling the distribution of both oxygen and nitrogen atoms directly at the TiN/HfO_2 interface.

With the addition of the Gd_2O_5 -layer, the oxygen concentration depth profile was derived both by means of electron energy loss spectroscopy (EELS) and atom probe tomography (APT). Structural investigation by means of high resolution transmission electron microscopy (HR-TEM) concluded the detailed study of the metal/dielectric interface.

MM 31.19 Wed 17:15 P5

Simulation of structural transitions in NiTi systems — •Daniel Mutter and Peter Nielaba — University of Konstanz, 78457 Konstanz, Germany

In this work, we performed atomistic molecular dynamics simulations of the structural phase transition in NiTi alloys between B19' at low and B2 at high temperatures [1]. To this end, a semi-empirical potential from the literature was adopted [2] and modified, which is based on the tight-binding model in second moment approximation. We present an analysis of crystallography and energetics of the emerging structures during a heating-cooling cycle, which is applied to systems with 2048 atoms under periodic boundary conditions. The experimentally known strong dependence of transition temperatures (TTs) on alloy composition is confirmed and related to an increasing lattice instability, arising when the perfect ordered composition with 50% Ni and 50% Ti is changed slightly. By applying free boundary conditions, spherical NiTi nanoparticles with diameters between 3 and 17 nanometers were simulated, where a size dependence of the TTs was observed. In order to explain this behavior, an order parameter for distinguishing locally between B19' and B2 was constructed, with which a visualization of the phase transition was possible, showing that the start of the structural transformation is mainly triggered by the surface of the nanoparticle.

[1] D. Mutter and P. Nielaba, Phys. Rev. B 82, 224201 (2010).
[2] W.S. Lai, B.X. Liu, J. Phys. Cond. Mat. 12, L53-L60 (2000).

MM 31.20 Wed 17:15 P5

Interaction of ultrashort XUV pulses with bulk magnesium — •Naira Grigoryan, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

A recently published experimental work (Nagler et al.) shows that the excitation of a material with very intense femtosecond XUV pulses first leads to an exotic state characterized by a very high density of core holes (about 1 core hole per atom) and relatively warm electrons. The next step is the formation of warm dense matter. In this work we perform all-electron ab-initio calculations to determine the main pathways from solid to warm dense magnesium. We simulate the XUV excitation by constructing a state with hot electrons and core holes. By analyzing particular optical and acoustic phonon modes at high symmetry points of the Brillouin zone in the highly excited electronic state as a function of the electronic temperature and the number of core holes we obtain an indication of the atomic pathways involved in the first stages of the formation of warm dense matter.

MM 31.21 Wed 17:15 P5

X-ray Raman Scattering Studies of Si-based Compounds Under Extreme Conditions — •Christoph Sahle[1], Christian Sternemann[1], John Tse[2], Max Wilke[3], Christian Schmidt[3], Alexander Nyrow[1], Julien Dubrail[3], Valentina Giordano[4], Laura Simonelli[4], Serge Desgreniers[5], and Metin Tolan[1] — [1]Fakultät Physik/DELTA Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany. — [2]Department of Physics, University of Saskatchewan, Saskatoon S7N0W0, Canada. — [3]Geoforschungszentrum Potsdam, Telegraphenberg, 14773 Potsdam, Germany. — [4]ESRF, Rue Jules Horowitz, 38043 Grenoble Cedex, France. — [5]Laboratoire de physique des solides denses, University of Ottawa, Ottawa K1N6N5, Canada.

The *in situ* study of low Z elements' absorption edges under extreme conditions is only feasible using hard x-rays. Here, non-resonant x-ray Raman scattering as an energy loss technique enables one to choose the energy of the primary x-ray beam freely and thus gives access to shallow absorption edges of samples in highly absorbing sample environments, e.g. diamond anvil cells, which do not permit electrons and soft x-rays as probe. Here, we present two studies of Si-based compounds under extreme conditions: a high pressure study of the peculiar phase transitions in silicon clathrate Ba_8Si_{46} via measurements of the Ba N_{45} and Si L_{23} edges. In addition, we present the first *in situ* high pressure – high temperature study at the Si L_{23} and Na L_{23} edge on hydrous $Na_2Si_3O_7$ melt, which may serve as a model for geologically relevant hydrous silicate melts in the deep earth.

MM 31.22 Wed 17:15 P5

Towards the study of electric field gradients in M_2AlC (M = Ti, Nb, V, Cr) MAX phases — •Daniel Jürgens[1], Christoph Brüsewitz[1], Michael Uhrmacher[1], Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]Georg-August-Universität Göttingen, II. Phys. Inst., Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

Layered ternary carbides like Ti_2AlC and Nb_2AlC have attracted great attention in recent time. These materials belong to the MAX phase family whose compounds show an unique combination of both metal- and ceramic-like properties. Some features are their excellent thermal and electrical conductivity even at high temperatures, their low density and high oxidation resistance as well as their easy machinability. The purpose of this work is to describe and understand their physical behavior on atomic scale since many investigations came to the conclusion that the observed characteristics on the mm or even μm scale have their origin in the microstructure. To do so the technique of perturbed angular correlation (PAC) was used beside XRD to gain detailed information about the atomic environment. Radioactive ^{111}In ions, decaying by a γ-γ cascade, were implanted into the samples, sensing as *spies* their local surrounding via hyperfine interactions. This method was applied to Ti_2AlC, Nb_2AlC, V_2AlC and Cr_2AlC. In each

material an axially symmetric EFG was found with a characteristic quadrupole coupling constant ν_Q variing between 180 MHz and 260 MHz, which decreases linearly with increasing measurement temperature. This work is supported by the DFG under contract HO 1125/19-1.

MM 31.23 Wed 17:15 P5

Phase-field study of needle crystal fragmentation — •Marius Kist[1], Abhik Choudhury[1], and Britta Nestler[1,2] — [1]Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestr.30, 76133 Karlsruhe, Germany — [2]Institute of Reliability of Components and Systems(IZBS), Karlsruher Institut für Technologie, Haid-und-Neu-Str.7, 76131 Karlsruhe, Germany

We investigate the melting process of a single solid phase in contact with its liquid for the case of a binary alloy at near to equilibrium conditions by two and three dimensional simulations based on a phase-field method. In particular, we study the effect of surface energy anisotropy on the melting behavior. In 2D, for the case of isotropic surface energies, the solid phase melts continuously keeping its shape intact. For the case of anisotropic surface energy giving rise to elliptical needle crystals, we observe a discontinuous melting behavior where, beyond a critical aspect ratio (major axis/minor axis), the needle splits into two fragments while melting. We investigate this phenomenon, and suggest a mechanism for its occurrence. In 3D, the classical Rayleigh-Plateau-Instability is known to cause a break up of a cylindrical surface into a row of droplets through surface energy minimization. This instability is an additional contribution to the splitting behavior of needle crystals. We study the interplay of the mechanisms of needle breaking in 2D and analyze the effect of Rayleigh Instability in the presence of bulk diffusion in 3D. From the phase-field simulations, we derive the time exponent for the kinetics of the needle crystal fragmentation.

MM 31.24 Wed 17:15 P5

Ti-based dendrite - nano/ultrafine eutectic composites: microstructure control via semi-solid processing — •Olga Shuleshova[1], Norbert Mattern[1], Wolfgang Löser[2], and Jürgen Eckert[1,3] — [1]Institute for Complex Materials, IFW Dresden, Germany — [2]Institute for Solid State Research, IFW Dresden, Germany — [3]Institute of Materials Science, TU Dresden, Germany

Recently, considerable advances are achieved in ductilization of the inherently brittle high-strength materials, such as metallic glasses and nano/ultrafine eutectics, through incorporation of soft dendritic phase, which primarily solidifies from the melt and is subsequently embraced in a strong matrix. An enhanced mechanical properties results from cooperative interplay of the inhomogeneous microstructure with the different deformation mechanisms of the respective phases, and thus are inherently related to the volume fraction, spatial sizes, morphology and overall distribution of the ductile crystalline phase reinforcement. Present work explores the possibility to control these parameters via isothermal holding between the liquidus and solidus temperature followed by rapid cooling of the semi-solid mixture. Previously applied only for the metallic glasses composites this approach is adopted here for the Ti-Fe-(Nb) system, known to form nano/ultrafine eutectic at moderate cooling rates. Moreover, relative simplicity of this system allows to study the peculiarities of the microstructures accessible via semi-solid processing in tight connection with the high-temperature phase equilibria given by thermodynamic description of the corresponding systems.

MM 31.25 Wed 17:15 P5

Differences of the evaporation field in dependence of the crystallographic direction in Al and W by means of Atom probe tomography — •Torben Boll[1,2] and Talaat Al-Kassab[1,2] — [1]Division of Physical Sciences and Engineering King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In field ion microscope (FIM) images the dependence of the brightness of the crystallographic direction is easily observed. This difference in brightness can be related to the evaporation fields at different poles. However this approach allows only a rough qualitative estimation. In this paper an approach will be presented, which utilizes the newly available Wide Angle Atom Probe Tomography (WA-APT) to identify quantitative relations.

The method will be discussed for pure Al- and W-samples. The results are relevant for the development of reconstruction algorithms in WA-APT. Current instruments can analyze a projection angle of about 70° compared to 20°, which was state of the art 10 years ago. Thus the assumption of hemispherical, symmetrical tips for the reconstruction is not valid anymore. Evaporation fields can be used to identify a complex tip shape and lead to more accurate reconstructions.

MM 31.26 Wed 17:15 P5

Micro-fabricated arrays of SU-8 capillaries with electroplated front electrodes — •Katharina Huhn, Markus Piechotka, Torsten Henning, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

We manufactured thin capillaries out of the negative resist SU-8 with multiple step photolithography. To avoid the formation of stress cracking, a special photomask pattern was designed. The inner diameter of the capillaries varied from 10 to 20 microns whilst the height was in the range of 40 to 100 microns. Afterwards a metal grid structure was deposited onto the top surface of the capillaries using evaporation and lift-off techniques as well as electro-plating.

The aim of this work is to study the feasibility of this method to produce an ionic liquid emitter. SU-8 with its high aspect ratio and easy handling suits the required conditions well. Additionally, SU-8 provides an electric isolating behaviour as needed.

To investigate the shape accuracy and possible defects we used optical, atomic force (AFM) as well as scanning electron microscopy (SEM).

MM 31.27 Wed 17:15 P5

Study of the silver ion release from antimicrobial nanosilver (nAg)/PTFE two dimensional (2D) model — •Nisreen Alissawi[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Dieter Garbe-Schönberg[2], and Franz Faupel[1] — [1]Institute for Materials Science-Multicomponents Materials, Christian-Albrechts-University, Kaiserstr.2, 24143, kiel — [2]Dept. of Geology/ ICPMS Lab, CAU Kiel, Ludewig- Meyn-Strasse 10, 24118 Kiel

Despite the great interest in silver based antimicrobial nanocomposites, it is still not clear how the composite morphology (nanoparticle size, concentration, and distribution) affect the mechanism and kinetics of the interfacial ion transfer reactions of the Ag nanoparticles due to the fact that metal nanoparticles embedded in a polymeric matrix are not directly accessible concerning their interfacial structure and reactivity. This problem will be approached in our present work by the usage of well defined model systems consisting of 2D nanoparticle arrays which are either directly accessible or covered by polymer barrier. The Ag nanoparticles and the PTFE polymer layers were synthesized by physical vapor deposition (PVD) techniques. The samples' morphology, optical properties and composition were examined by Transmission Electron microscopy (TEM), UV-Visible Spectroscopy (UV-Vis) and X-Ray Photoelectron Spectroscopy (XPS), respectively, and the time-dependent release of silver ions after inserting in water was measured using Inductively coupled plasma mass spectrometry (ICP-MS). Time dependence of silver ions release on the particle size and barrier properties are discussed.

MM 31.28 Wed 17:15 P5

Shear-stress induced grain boundary motion in nanocrystalline $Pd_{90}Au_{10}$ — •Manuel Grewer[1], Aaron Weis[2], and Rainer Birringer[1] — [1]Universität des Saarlandes FR 7.2 Experimentalphysik, Saarbrücken, Deutschland — [2]Karlsruher Institut für Technologie - Institut für Nanotechnologie, Eggenstein-Leopoldshafen, Deutschland

The role of shear stress as a driving force for grain boundary migration is a topic which is currently attracting much attention [1,2]. The miniaturized shear compression specimen [3] is a versatile tool to impose large shear deformation during mechanical testing. This shear deformation is strongly localized in the gauge section of the test specimen. Thus it provides an appropriate testing geometry to study grain boundary migration in nanocrystalline materials under dominant shear stress. We investigate the evolution of the grain size distribution function, which has been derived from TEM dark field images, before and after plastic shear deformation of nanocrystalline $Pd_{90}Au_{10}$ with an initial grain size of 10 nm. We find clear evidence for shear deformation driven grain boundary migration at room temperature and >15% plastic strain.

[1] J.W. Cahn et al., Acta mater. 54 (2006), 4953-4975, [2] T.J. Rupert et al., Science 326 (2009), 1686-1690, [3] M. Ames et al., Mater. Sci. Eng. A 528 (2010), 526-532

MM 31.29 Wed 17:15 P5

Thermal stability of indium nanoparticles embedded in an aluminum matrix — •Mostafa Mohamed, Martin Peterlechner, Joachim Bokloh, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University Münster, 48149 Münster,Germany

The thermodynamics of nanoscaled systems have drawn considerable scientific attention due to the strong influence of the particle size and shape. In the present work, nanoparticles of indium embedded in an aluminum matrix were processed by rapid quenching using the melt-spinning technique. The as-processed samples were analyzed using conventional and analytical transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). TEM data revealed isolated and mainly spherical nanoparticles of indium with a size in the range of 20 to 300 nm. Indium particles in aluminum grains are equiaxed, whereas particles at aluminum grain boundaries show elongation. Analytical TEM showed neither a notable concentration of indium in the aluminum matrix nor a concentration gradient at the interfaces of the particles. By DSC experiments using a wide range of different constant heating and cooling rates, broad melting and crystallization peaks were observed. A slight reduction of the melting temperature of the embedded particles in comparison to the bulk indium is detected, whereas the crystallization temperature shifts to remarkable low temperatures. Upon thermal cycling, the melting as well as the crystallization temperatures of the nanoparticles reduces and the peak shape changes clearly.

MM 31.30 Wed 17:15 P5

Modelling of pine-tree nanowires — •Rainer Schulz[1,2] and Robert Spatschek[1] — [1]Max-Planck Institut für Eisenforschung GmbH, Düsseldorf — [2]ICAMS, Ruhr-Universität Bochum

Nanowires are thin wires (e.g. metal) which are severely restricted in 2 dimensions of space and show a one-dimensional quantization of conductivity. They have a length to diameter ratio of about 1000 and a thickness of some nanometers. Often, they grow defect-free in a catalytic reaction from a substrate, but recently interesting patterns have been observed in situations, where the wires grow in a controlled way with a screw dislocation inside the trunk. As had been predicted earlier, this leads to the so called Eshelby twist of the wire, which stabilizes the dislocation in the center of the wire, and experimental findings suggest that this torsion favors the emergence of sidebranches. In this study we use finite element methods and Ginzburg-Landau models to investigate the dislocation motion and morphology evolution of the nanowire numerically and compare the results to theoretical predictions.

MM 31.31 Wed 17:15 P5

Synthesis and characterization of functional metal oxide nanowires — •babak nasr, subho dasgupta, di wang, robert kruk, and horst hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, D-76344 Eggenstein-Leopoldshafen,Germany

Semiconducting metal oxide nanowires (NWs) like SnO2, In2O3, ZnO have found a wide range of applications in electronic devices, such as varistors, gas sensors and lithium ion batteries. Doping with appropriate elements, such as indium (In), antimony (Sb) and tantalum (Ta) can change their optical and electrical properties. In this work undoped and doped SnO2 NWs were synthesized on (100) Si substrates by a catalyst-mediated vapor-liquid solid (VLS) process. Tin oxide*indium oxide NWs were successfully obtained at a constant gas flow rate (O2 1% and Ar, 99%, 100 sccm), 800*900°C temperature window and a growth time of 10 min. The impact of catalyst size on NW*s thickness was studied and it was found that smaller catalyst particles result in thinner NWs. The thickness of NWs was evaluated through scanning electron microscopy (SEM). The crystallographic structure, single crystallinity and growth direction were studied using X-ray diffractometry (XRD) and high-resolution*transmission microscopy (HRTEM) respectively. Well-defined lattice fringes suggested the growth direction along [101]. Compositional analyses via x-ray photoemission spectroscopy (XPS) and Rutherford backscattering spectroscopy (RBS) showed the presence of Sn and Sb as dopant. The NWs were aligned on a patterned substrate for further electrical characterization.

MM 31.32 Wed 17:15 P5

Magnetoconductivity of ferromagnetic thin film samples probed by scanning microwave microscopy — •Stephan Streit[1], Ferry Kienberger[2], Hans-Peter Huber[2], Matthias Fenner[3], Heidemarie Schmidt[1], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden — [2]Agilent Technologies Austria GmbH, Aubrunnerweg 11, A-4040 Linz, Austria — [3]Agilent Technologies Inc., 61476 Kronberg, Germany

Due to the miniaturisation of electrical devices, measurement techniques need to keep pace to achieve an appropriate spatial resolution. Scanning Microwave Microscopy (SMM) [1] offers the possibility to combine impedance measurements with the advantages of atomic force microscopy. In our work we use a SMM in contact mode to investigate the magnetoconductivity of ferromagnetic thin films. The samples have been prepared by electron beam deposition of iron, cobalt, or nickel films and a Cr protection layer on ZnO substrates. Our quantitative simulation is based on the dependence of the microwave reflection coefficient S11 on conductivity and permeability of ferromagnetic materials [1]. The influence of multiple microwave reflections [2] on the S11 coefficient has been tested for 10 and 20 nm thick ferromagnetic films.

[1] H. Melikyan et al., Ultramicroscopy 108 (2008) 1030-1033 [2] D.M. Pozar, Microwave Engineering, Wiley&Sons, 2005

MM 31.33 Wed 17:15 P5

Influence of the preparation technique on the temperature induced phase separation and nanocrystal formation in $Si_xGe_yO_z$ — •Alexander Nyrow[1], Alexander Schwamberger[1], Christoph J. Sahle[1], Christian Sternemann[1], Achim Hohl[2], Patrick Degen[3], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Experimentelle Physik Ia, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Institute for Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — [3]Physikalische Chemie II, Technische Universität Dortmund, Otto-Hahn-Str. 6, 44227 Dortmund, Germany

Since the discovery of visible luminescence from nanocrystallized Si in the early 90s, the study of group IV semiconductor/oxygen systems has received great attention. Due to their unique electronic properties Ge and Si nanocrystals (NCs) are promising candidates for, e.g., light emitting diodes or fast and stable non-volatile flash memory devices. Despite the intensive research regarding the electrical and optical properties of nanoparticles embedded in oxide matrices, spectroscopic studies of its formation process are rare. The NC formation is induced by thermal annealing of the amorphous precursors. It is already known that the composition and the local structure of $Si_xGe_yO_z$ and thus the phase separation essentially depend on the preparation process. To investigate the influence of the preparation technique on the NC formation, samples with various Si/Ge ratios were prepared by evaporation of GeO_2 and Si and by thermal processing of polymers derived from phenyl trichlorogermane and phenyl trichlorosilane, respectively.

MM 31.34 Wed 17:15 P5

Influence of magnetic gradient fields on the electrodeposition of metallic layers — •Kristina Tschulik[1,2], Franziska Karnbach[1], Ralph Süptitz[1,2], Margitta Uhlemann[1], Annett Gebert[1], and Ludwig Schultz[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany

With regard to surface finishing electroplating from aqueous solutions is a very common method. It is well-known, that by superposition of homogeneous magnetic fields the deposition process as well as morphology, texture and magnetic properties of deposits can be changed due to Lorentz force induced convection. Additionally, it has been shown that non-homogeneous magnetic fields are able to increase deposition rates dramatically due to the Magnetic field gradient force acting on paramagnetic ions. However, effects of magnetic gradient fields on deposit properties are still not well investigated, although interesting results due to interaction of Lorentz force and Magnetic field gradient force might be expected.

Hence, this work is focused on externally applied, well-defined magnetic gradient fields and their impact on deposition behavior and deposit properties. It has been found that structured deposits and significant diversification of roughness and grain structure can be observed. Effects of the involved magnetic forces are considered in order to propose a structuring mechanism, which bases on magnetically induced local convection.

MM 31.35 Wed 17:15 P5

Ab initio simulation of coherent phonons in BN-nanotubes — •Bernd Bauerhenne, Eeuwe S. Zijlstra, and Martin E. 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. An intense ultrashort laser pulse excites the electronic system to very high temperatures, whereas the ions remain close to their initial state. The ensuing laser-induced processes of electronic origin include bond softening, phonon frequency changes (hardening or softening), and the excitation of coherent phonons. We study these processes by means of large-scale molecular dynamics simulations based on density functional theory, including levels of excitation where the nanotube breaks. Our results show a strong radial breathing mode, increasing in amplitude with the laser-induced electronic temperature. We also determine the damage threshold.

MM 31.36 Wed 17:15 P5

Nano-morphology of optoelectronic circuits exploiting focused ion beam lithography — Selcuk Zorlu[1], •Hideyuki Maki[1,2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TUM Garching, Germany — [2]Department of Applied Physics and Physico-Informatics, Keio University, Hiyoshi, Yokohama, Japan

We present studies on the nano-morphology of optoelectronic circuits by exploiting a focused ion beam (FIB) lithography in combination with an electron beam microscope. To this end, lamellas of optoelectronic circuits are fabricated in a cross-beam (FIB and e-beam) microscope. The lamellas are side-cuts of the circuits, and they give access to the vertical structure of the semiconducting, metal, or organic layers. The presented method allows analyzing interpenetrating networks of vertical, optoelectronic two-terminal circuits.

MM 31.37 Wed 17:15 P5

Pore lattice deformation of silica nanochannels (SBA-15) during uptake and release of solid and liquid argon — •Daniel Rau[1], Dirk Wallacher[2], Gerald Zickler[3], Patrick Huber[1], and Rolf Pelster[1] — [1]FR 7.2 Experimentalphysik, Universität des Saarlandes, Germany — [2]Helmholtz Zentrum Berlin, Germany — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität / University of Leoben, Austria

We have studied the structural change of cylindrical, hexagonally ordered silica nanopores (SBA-15) as a function of their filling with solid and liquid argon, respectively. Sorption isotherms were measured at 71.5 K (solid) and 81.5 K (liquid). Simultaneously the material was characterized via small-angle-X-ray-scattering (SAXS) using synchrotron radiation at the Hasylab (DESY/Hamburg). In this way we are able to evaluate the deformation of the pore lattice during adsorption and desorption.

MM 31.38 Wed 17:15 P5

Synthesis of ZnO core spike particles as composite fillers with a high throughput method — •Sebastian Wille, Tönjes Koschine, Christoph Chluba, Stefan Freitag, Yogendra Kumar Mishra, and Rainer Adelung — Funktionale Nanomaterialien, CAU Kiel

ZnO core spike particles are typically micro particles covered with nanoscopic spikes. They show advanced properties compared to conventional fillers like roundish particles and short fibers. An example is a very strong mechanical interlocking behaviors. This property together with its hardness makes this material very interesting for compounds with enhanced mechanical properties. In addition ZnO has very interesting electric and electronic properties, which make the range of possible applications for composites containing ZnO core spike particles very wide. In order to use ZnO core spike particles as filler for bulk materials, considerable amounts are necessary. A problem during the oxidation based synthesis of such particles using Zn-powder as source material is the separation of the single Zn-particles, which is necessary for oxygen supply, for avoiding sinter processes and allowing the nanoscopic spikes to grow. We introduce simple processing routes found as solution for this problem. Large amounts of microscopic Zn-powder can be converted to ZnO core spike particles with a total size from nanometers up to a couple of micrometers. Furthermore by changing the growth parameters it is also possible to modify the particle shape.

MM 31.39 Wed 17:15 P5

DFT studies of clusters and nanowires in external fields — •Marcus Beck, Gary Klindt, Manuel Matt, and Peter Nielaba — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

Density functional theory (DFT) studies on the stability and structural properties of small clusters and nanowires are performed. One point of interest is the arranging of diverse Si nano clusters. We use external electrostatic fields for ordering purposes of these clusters by polarization effects. We further investigate the $Al_{13}H$ cluster with distorted icosahedral formed Al_{13} which has several isomers with different positions of the hydrogen atom. We analyze the effects of electrostatic and magnetic fields on these systems in order to explore the possibility to switch the isomers by external fields. The geometrical configuration of monoatomic Au nanowires and the structural change due to an external electric field is also part of our investigations. Distances, angles and binding energies are influenced by the field and therefore breaking of the nanowire is more likely. These changes may influence the conductance of the wire substantially which we study using the non equilibrium Greens function formalism (NEGF).

MM 31.40 Wed 17:15 P5

Laser-assisted atom probe tomography of self-organized surface layers — •Andreas Stoffers and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

The availability of femtosecond lasers facilitates the analysis of new material classes by atom probe tomography. Pulsed-laser atom probe tomography (PLAP) has the potential to give even structural and chemical information of biological and organic materials at an atomic scale. In order to explore the possibilities of analyzing nanometric materials, we have chosen the model cases of polyelectrolyte multilayers (PEM) and self assembled monolayers (SAM). PEMs are adsorbed step by step as a multilayer of poly-anions and poly-cations at the apex of sharp gold tips. SAMs are also adsorbed in a self-assembling process at the apex of sharp gold tips, but offer only a limited volume for analysis. By means of laser-assistance it is indeed possible to chemically analyze different PEMs and SAMs. In all cases the mass spectra are complex, characterized by peaks of multiple fractions of different molecular mass. Since these molecular species are very similar for the studied polymer types, it is hard to distinguish the organic molecules from the time-of-flight spectrum. However, different polymer-types might be distinguished based on the intensity ratio between characteristic mass peaks. In addition, a 3D reconstruction of a fluorinated SAM will be presented to demonstrate the ability of getting structural information of the alignment and distribution of the oligomeres.

MM 31.41 Wed 17:15 P5

Spin wave modes in magnetic nanostructures as seen by Ferromagnetic Resonance — •Sven Stienen, Ralf Meckenstock, Christoph Hassel, Jürgen Lindner, Nathalie Reckers, and Michael Farle — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

Micromagnetic simulations using the 3D Object Orientated Micromagnetic Framework (OOMMF) software were performed for a permalloy (Py) stripes arranged in a the form of crosses. In difference to most previous work, we apply a small time-dependent magnetic field with a fixed frequency (10GHz) to simulate the microwave field used in ferromagnetic resonance (FMR). Different spin wave excitations like the uniform, edge and not-aligned modes can be identified and visualized in time and space. In the simulation an external in-plane angular dependent magnetic field is varied between 0mT and 400mT yielding spectra as in the experimental ferromagnetic resonance. These simulated spetra are compared to experimental spectra of structured samples. Our simulation yields visualizations of the distribution of the excitation inside the stripes thus unambiguously identifying more than 10 different modes occurring in the stripes. These simulated images and spectra are helpful to find the best conditions for locally resolved ferromagnetic resonance measurements. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB 491.

MM 31.42 Wed 17:15 P5

Phase-field Modeling of Twin Boundary Motion in Magnetic Shape Memory Alloys — •Christian Mennerich, Frank Wendler, Marcus Jainta, and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Magnetic shape memory (MSM) alloys have gained high interest in the last decade. As actuators, they provide fast response times and low energy costs in operation. When in the low temperature martensitic state, large recoverable strains (more than 6% in Ni_2MnGa-based alloys) can be achieved in these ferromagnetic hard materials by control-

ling the motion of twin boundaries by applying an external magnetic field.

Using a multi-phase field model of Allen-Cahn type basing on a Helmholtz free energy density formulation, the microstructure rearrangement in Ni_2MnGa is described. Order parameters, related to the different eigenstrains of the twin variants, describe their time-spatial evolution, depending on energy contributions for twin interfaces and bulk phase states (including micromagnetic and magneto-elastic energies). Assuming an isothermal setting below the Curie temperature and the martensitic start temperature, we can solve for the elastic displacement field (damped wave equation) and the volume averaged magnetization (Landau-Lifshitz-Gilbert equation using a geometric integration scheme). We show results of simulations of the reversible transformation process in single crystals, and we propose an extension of the model to polycrystalline settings. The coupled evolution of twin variants and magnetic domains is investigated in more detail, and the resulting magnetic domain structure is visualized.

MM 31.43 Wed 17:15 P5

TEM Investigations on NiMnInCo and Fe70Pd30 Ferromagnetic Shape Memory Alloys — •Burak Erkartal[1], Andriy Lotnyk[1], Viola Duppel[2], Robert Niemann[3], Christoph Bechtold[4], Christiane Zamponi[4], Sebastian Fähler[3], Ludwig Schultz[3], Eckhard Quandt[4], and Lorenz Kienle[1] — [1]Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart — [3]IFW Dresden, P. O. Box 270116, 01171 Dresden — [4]Inorganic Functional Materials, CAU Kiel, Kaiserstr. 2, 24143 Kiel

NiMnInCo meta-magnetic shape memory alloys have attracted considerable interest because they can be utilized for the magnetocaloric effect. Here we focus on TEM investigations of an epitaxially grown NiMnInCo thin film sputtered on (001) oriented MgO substrate with Cr buffer layer. Besides the presence of 6M, 7M modulated martensites, structural analysis by precession electron diffraction confirm also a non-modulated tetragonal phase. EDX elemental maps recorded on a cross-section indicate defects of the Cr buffer layer at the interface. Additionally, columnar regions with lower In content were observed. Further interest was concentrated on Fe70Pd30 due to the exceptional strain in response to a variation of a moderate magnetic field. Fe70Pd30 was deposited by magnetron sputtering on (001) MgO substrates coated with different metallic buffer layers. HRTEM micrographs and diffraction patterns confirm the tetragonal single crystal growth of the Fe70Pd30 films of ˜1.2 micrometer thickness. The authors thank the DFG for funding via the SPP 1239.

MM 31.44 Wed 17:15 P5

Low-temperature relaxation in NiTi-based shape memory alloys — •Joan Torrens-Serra, Daniel Salas, Eduard Cesari, and Sergey Kustov — Departament de Física, Universitat de les Illes Balears, cra. de Valldemossa km 7.5, E-07122, Palma de Mallorca, Spain

We have studied the structural changes occurring in different Ni-Ti and Ni-Ti-Fe alloys over the temperature range from 13 to 300 K by means of mechanical spectroscopy, calorimetry (DSC) and electrical resistivity measurements. Several binary and ternary alloys were used with different thermal and mechanical history, which demonstrate distinct transformation paths: B2-B19', B2-R and B2-R-B19'. Temperature dependence of the internal friction (IF) was studied over the range 90-137 kHz for different strain amplitudes from 3*10E-7 to 5*10E-5. In addition to the martensitic and intermartensitic transformations, the IF curves showed a peak at about 90 K in annealed and water-quenched samples independently of their composition which can not be detected by DSC or electrical resistivity measurements. The thermally activated nature of the relaxation has been confirmed using different measurement frequencies. Since the IF peak is observed for ultrasonic frequencies at temperatures of around 90 K, it corresponds to a new relaxation phenomenon, not reported so far in Ni-Ti family of alloys, with the activation energy of the order of only 0.01 eV. On the other hand, no relaxation is found in deformed alloys not subjected to annealing heat treatments. The origin of this relaxation may be attributed to the presence of interstitial hydrogen atoms.

MM 31.45 Wed 17:15 P5

The effect of cooling rate on undercooling of pure Sn single drop — •Bin Yang[1], Yulai Gao[2], Alexander S. Abyzov[3], Evgeny Zhuravlev[1], Jürn Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Shanghai Key Laboratory of Modern Metallurgy & MaterialsProcessing, Shanghai University, China — [3]National Science Center, Kharkov Institute of Physics and Technology, Ukraine

The cooling rate dependence of undercooling of pure Sn single drop is studied by the non-adiabatic fast scanning calorimetry in a large range of cooling rate spanning four orders of magnitude. The experimental results and theoretical analysis show that the undercooling can be obviously increased first with increasing cooling rate going over to a stage of slow increase for high cooling rates, which indicates a shelf-like dependence of undercooling on cooling rate before and after a "crossover" at higher cooling rate where two different heterogeneous mechanisms act simultaneously.

MM 31.46 Wed 17:15 P5

Computational approaches to compute interface tensions γ_{lw} and γ_{cw} for colloidal systems — •Debabrata Deb, Alexander Winkler, Peter Virnau, and Kurt Binder — Johannes-Gutenberg-Universität, Staudinger Weg 7, 55099 Mainz, Germany

On this poster we present recent efforts to calculate interface tensions γ_{lw} between liquid and wall and γ_{cw} between crystal and wall for hard spheres and the effective Asakura-Oosawa model. Wall interactions are modelled with the purely repulsive Weeks-Chandler-Andersen potential. Several approaches are tested: A method based on the anisotropy of the pressure tensor for γ_{lw}, a recent approach to compute absolute free energies proposed by Schilling and Schmid [1], and a thermodynamic integration based on slowly moving the system away from the bulk towards the confined state.

[1] T. Schilling and F. Schmid, J. Chem. Phys **131** (23), 231102 (2009)

MM 31.47 Wed 17:15 P5

Determination of the pressure activation volume via the deformation of nanocrystalline PdAu-samples with different shear-compression-ratios — •Christian Braun and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

The recently introduced miniaturisation of the shear-compression-specimen [1] allows the mechanical testing of small samples such as inert gas condensed nanocrystalline materials via a dominant shear-deformation. The stress-strain-curve and further parameters as strain components or hydrostatic pressure P are calculated by FEM-simulations based on the experimental force-displacement-diagram. By means of a variation of the shear-angle, it is possible to vary the shear-compression-ratio and the hydrostatic pressure P in the deformation zone. This permits the determination of the differential quotient $\partial\sigma/\partial P$ which is necessary to calculate the pressure activation volume Δv_P given as $\Delta v_P = \frac{\partial\sigma}{\partial P}\Delta v_\sigma$, where Δv_σ is the shear activation volume obtained from stress-strain-curves taken at different strain rates [2]. On this poster we present first simulation results for the expected variation of P for different shear angles as well as first experimental findings measured at nanocrystalline $Pd_{90}Au_{10}$-samples with an average grain diameter of about 10 nm.

[1] M. Ames, J. Markmann, R. Birringer, Mater. Sci. Eng. A 528, 526 (2010), [2] A.S. Argon, Strengthening Mechanisms in Crystal Plasticity, OUP (2007)

MM 31.48 Wed 17:15 P5

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

The mechanical properties of nanoscale metals differ from those of macroscale samples, especially the increasing strength with decreasing sample size. In this work, the stress-strain behavior of single crystalline Au nanowires with diameters between 40 and 200 nm are studied using an instrumented tensile stage in an SEM. The wires are transferred from the growth substrate to the tensile stage without deforming them using a micromanipulator. Displacements are applied by a piezoelectric based actuator while forces are measured with a capacitive MEMS device. All tested wires show an initial elastic regime with a slope of around 68GPa, which is reversible on unloading. This is followed by a gradual onset of plasticity and eventually by fracture after a plastic strain of 1 to 3%. The failure stresses, which reach up to 1.2GPa, confirm the trend that smaller samples have higher flow stresses than bulk materials. Investigations of the failed wire segments, which were transferred subsequently to a TEM grid, confirm the size-dependent deformation mechanisms observed during in situ TEM tensile testing,

namely that deformation proceeds by partial dislocation motion rather than full dislocation motion below a critical size of approximately 180 nm.

MM 31.49 Wed 17:15 P5

Effect of hydrogen on the multiplication of dislocations in cold-rolled palladium — •Hans Peter Barth, Yuzeng Chen, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

According to a novel defectant (defect acting agents) concept (R. Kirchheim, IJMR (Z. Metallkde) 100 (2009) 483 and Acta Materialia 55 (2007) 5129 and 5139), the solute-defect interaction in materials can reduce defect formation energies. In the present work, the influence of hydrogen (defactant) on the multiplication of dislocations in cold-rolled palladium is studied. Palladium is used as a model system because it offers a sufficient hydrogen solubility and fast hydrogen diffusion. Well annealed palladium was electrochemically charged with different amounts of hydrogen ($\leq$1at%) and subsequently cold-rolled to a certain deformation degree. Pure palladium was also cold-rolled to the same deformation degree for comparison. Afterwards, the hydrogen was electrochemically uncharged from the deformed samples. Dislocation densities were studied by means of XRD and electromotive force (EMF) measurements during hydrogen recharging. Compared to pure palladium, X-ray profiles of samples charged with hydrogen prior to deformation exhibit more significant Bragg peak broadening, indicating higher dislocation densities. EMF measurements confirm the conclusion from the XRD measurements. Both methods suggest hydrogen can facilitate the multiplication of dislocations in palladium. Apart from the above results, a new experimental setup for in-situ EMF measurements during tensile tests will be shown.

MM 31.50 Wed 17:15 P5

Die Bonner Positronen Mikrosonde - ein vielfältiges Werkzeug für die Materialforschung — •Niels Lennart Raeth[1], Olga Herdt[1], Meng Liu[1], Benedikt Klobes[1], Matz Haaks[1], Karl Maier[1] und Christoph Hugenschmidt[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, 53115 Bonn — [2]FRM II und Physik Department E21, Technische Universität München

Die Bonner Positronen Mikrosonde (BPM) erzeugt einen fein fokussierten Positronenstrahl mit einstellbarem Strahldurchmesser von 1 - 200 μm und besitzt ein integriertes Rasterelektronenmikroskop (REM). Proben können so lateral hochaufgelöst mit den Methoden der Positronenannihilationsspektroskopie (PAS) untersucht werden und man erhält Zugang zur detaillierten Messung von Plastizität und Defektdichten verschiedenster Materialien.

Instrumentell ist eine Weiterentwicklung der BPM im Bereich der Strahlfokussierungs- und -justagesysteme geplant. Zudem soll die BPM um die Möglichkeit zur ortsaufgelösten Messung der Positronenlebensdauer ergänzt werden.

Der aktuelle Fokus der Forschung liegt auf schweißbaren Aluminiumlegierungen der Systeme AA5xxx und AA6xxx. Besonderes Interesse gilt hier der Defektkonzentration direkt an der Schweißnaht und in der angrenzenden Wärmeeinflusszone, vor allem im Hinblick auf eine PAS-basierte Schadensvorhersage für geschweißte Aluminiumwerkstoffe.

MM 31.51 Wed 17:15 P5

Tailoring the mechanical properties of nanocrystalline fcc metals: A Molecular Dynamics study on the effects of twins and miscible solutes on deformation processes — •Jonathan Schäfer, Alexander Stukowski, and Karsten Albe — TU Darmstadt, Darmstadt, Germany

For the presence of twins, a strengthening effect of nanocrystalline metals has been reported in experiment and simulation. For the case of miscible solutes, little is known about their effect on the structure and properties of nanocrystalline metals.

We present a comparative atomistic study on the effect of twins on the deformation behavior of nanocrystalline Cu and Pd. A new analysis method based on an automated Burgers circuit is applied, which allows us to analyze the dislocation interactions with twin planes and grain boundaries, and to directly measure dislocation, stacking fault, and twin boundary densities as functions of strain. We show, how a strengthening or softening effect of twins depends on the properties of a given fcc material i.e. its generalized planar fault energies.

For the case of Pd, we additionally show, how miscible solutes (Au) influence the behavior of our nanocrystalline structures in the elastic and plastic regime and why this depends on the distribution of the solutes. Here, samples are alloyed using a hybrid MD-MC method sampling the semi-grandcanonical ensemble. The automated Burgers search is applied as well and allows us to quantitatively compare the slip processes and planar faults as a function of composition and relaxation state.

MM 31.52 Wed 17:15 P5

Dynamics of small strain plasticity within the framework of a phase-field model — •Jan Höhn[1], Daniel Schneider[1], Alexander Vondrous[2], and Britta Nestler[1,2] — [1]Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology — [2]Institute of Materials and Processes, Karlsruhe University of Applied Science

A small strain plasticity model, based on the principles of continuum mechanics, was incorporated into a phase-field model for polycrystalline material systems in order to investigate the influence of plastic deformation on the change of the free energy. As a first approach, the Prandtl-Reuss model was implemented consisting of an associated flow rule in combination with the von Mises yield criterion and a linear isotropic hardening approximation. The fundamental set of equations is derived from an energy density functional and the numerical solution method is described. Simulations with simple loads on microstructures were performed illustrating the dynamic evolution of the stress and plastic strain by solving the momentum balance and by using a radial return mapping algorithm, respectively. An outlook on the long-term objectives of the new phase-field model is given ranging from applications to crack propagation, recrystallisation and annealing processes.

MM 31.53 Wed 17:15 P5

Examination of stress drops due to grain boundary motion in nanocrystalline PdAu-samples — •Michael Davis, Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

The miniaturized shear-specimen [1] allows one to examine the mechanical behaviour of nanocrystalline materials under dominant shear deformation. Due to the localisation of the plastic deformation in the gauge section, this samples geometry is particularly useful to study shear-stress driven grain boundary migration [2]. MD simulations predict a stick-slip-like deformation manifesting as stress drops in the force-displacement-diagram. In order to elucidate stick-slip behaviour, we probe the shear deformation in the gauge with high resolution optical displacement measurements. [1] M. Ames, J. Markmann, R. Birringer, Mater. Sci.Eng. A 528, 526 (2010), [2] J. W. Cahn, Y. Mishin, A. Suzuki, Acta Mat. 54,4953 (2006)

MM 31.54 Wed 17:15 P5

Mechanical characterization of chromium-based adhesion layers for hydrogenated amorphous carbon coatings — •Christoph Schmid, Jens Schaufler, Verena Maier, Karsten Durst, and Mathias Göken — Department of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, Germany

Hydrogenated amorphous carbon (a-C:H) coatings show unique properties, such as high hardness, low coefficients of friction and chemical inertness, which make them suitable for the application as wear protective coatings. At this the interfacial adhesion strength between steel substrates and the coating is a crucial point which often limits the reliability of coated components in high load applications. On an industrial scale metallic adhesion layers are a common technique to achieve a well adherent a-C:H coating. In this work, two chromium-based adhesion layers for a-C:H coatings with different adhesion qualities and a total thickness of less than 1 micron were investigated. By carrying out in-situ bending tests on FIB-milled micro-cantilevers in a SEM, the interface fracture strength between the adhesion layer and the a-C:H coating were determined quantitatively. Furthermore, nanoindentation tests on small angle cross sections (SACS) of the coating systems revealed information about the mechanical properties in terms of Hardness and Young's modulus. Performing auger-electron-spectroscopy on the SACS differences in the chemical gradients for the investigated adhesion layers can be found. With these results a correlation between the interfacial adhesion strength with the chemical composition and the mechanical properties of the coating systems can be given.

MM 32: HV Gandin

Time: Thursday 10:15–10:45 Location: IFW A

Invited Talk MM 32.1 Thu 10:15 IFW A

Direct simulation of in-situ real time X-ray solidification experiment — •Charles-André Gandin[1], Guillaume Reinhart[2], Nathalie Mangelinck-Noël[2], Henri Nguyen-Thi[2], Bernard Billia[2], and José Baruchel[3] — [1]MINES ParisTech, CEMEF CNRS 7635, Sophia Antipolis, F — [2]Aix-Marseille Université, IM2NP CNRS 6242, Marseille, F — [3]ESRF, Grenoble, F

In most metallic alloys, solidifying grains are made of a mixture of a dendritic solid, s, plus an interdendritic liquid, d. The grain envelope is delimited by the dendrite tips that grow in an extradendritic liquid, l. Due to segregation of solutal elements between the solid and liquid, the composition of the liquids are different. Mass exchange takes place between these liquids by diffusion and thermosolutal convection, leading to segregation patterns between the grains. Upon cooling, solidification ends with the formation of a eutectic structure. A model is presented to simulate the development of such structures and segregation patterns. A directional solidification experiment using Al - Ni is also presented. It is based on in-situ real time X-Ray imaging performed at the European Synchrotron Radiation Facility. While the dendritic grain structure and the eutectic front are resolved, access to the liquid flow is not possible and the composition field can so far only be qualitatively observed. The presentation will show how the use of the model can be conducted to help understanding the formation of the dendritic and eutectic structures by a direct simulation of the liquid flow and its interaction with the growing solid phases.

MM 33: Topical Session Electron Theory IV

Time: Thursday 11:00–13:00 Location: IFW A

Topical Talk MM 33.1 Thu 11:00 IFW A

Playground magnetism in low-dimensions: impact of first-principles theory — •Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Metals in reduced dimensions developed to a playground for interesting magnetic phenomena. In low dimensions, metals that are nonmagnetic in bulk can become magnetic in low dimension, magnetic interaction strengths are largely modified and magnetic anisotropies change by orders of magnitude. Nanostructures with lattices of increasing topological frustration can be grown leading to magnetic structure of unprecedented complexity. Magnetic structures can be modified by local probes. The choice of the substrate is an additional parameter that can modify the physics of these systems. In this presentation is shown, how systematic first-principles calculations based on the density functional theory carried out with innovative cutting edge electronic structure methods can unravel the physical trends in the high-dimensional phase space of low-dimensional magnets and how that inspires suggestions of new systems with unexpected physical phenomena.

Topical Talk MM 33.2 Thu 11:30 IFW A

Metallic and half-metallic magnetism — •Jürgen Kübler — Technische Universität, Darmstadt, Germany

The topic of the talk is introduced by means of two (rather old) examples, RhMn3 and Mn3Sn; these are metallic magnets that order in different non-collinear moment arrangements. Density functional theory explains their peculiar ground states and allows a determination of the exchange interactions that result in fairly good estimates of their ordering temperatures. Work by Fähnle et al. on a fast approach to the simulation of spin dynamics is extended to Heusler compounds, for which the half-metallic gap is discussed together with examples of spin-wave spectra and the role of spin-orbit coupling. Some variants of tetragonal Heusler compounds are discussed that have magnetic properties which make them interesting for spintronics applications.

Topical Talk MM 33.3 Thu 12:00 IFW A

Strain effects in magnetic and ferroelectric complex oxides from first principles — •Claude Ederer — School of Physics, Trinity College, Dublin 2, Ireland

For many applications complex functional oxides are epitaxially grown on substrates with slightly mismatched lattice constants. The resulting epitaxial strain can have drastic effects on the functional properties of the thin film materials, and in fact provides an attractive way to optimize ferroic properties or stabilize new phases. First principles electronic structure calculations are a powerful tool to investigate these effects, and also allow to separate genuine strain effects from other influences that are generally present in thin film samples.

In this talk I will discuss several examples of strain effects in complex oxides and I will present results of first principles calculations that allow to clarify the underlying mechanisms. In particular I will discuss the recently observed strain-induced morphotropic phase boundary in multiferroic $BiFeO_3$, the occurrence of strain-induced ferroelectric instabilities in the magnetic perovskites $CaMnO_3$ and $LaCrO_3$, and the effect of epitaxial strain on the magneto-crystalline anisotropy in the spinel ferrites $CoFe_2O_4$ and $NiFe_2O_4$.

MM 33.4 Thu 12:30 IFW A

Order and phase stability in CoPt: the role of magnetism. — •Sondes Karoui[1], Hakim Amara[1], François Ducastelle[1], and Bernard Legrand[2] — [1]LEM, ONERA-CNRS, BP72 92322 Châtillon Cedex, France — [2]SRMP, CEA, Saclay, France

Transition metal nano-alloys (FePd, CoRh, and CoPt) are innovative new materials whose size and chemical composition govern their physical and chemical properties. CoPt, the focus point of this study, had been duly studied in the bulk phase both experimentally and theoretically. There exists a large array of results that clearly hint at the importance of magnetism, and the stabilization that it brings to the system. Indeed, we strongly believe that the crystallographic order present in CoPt can be attributed to the alloy*s inherent magnetic character.

To point out this effect, Density Functional Theory calculations have been performed using the ABINIT code with and without magnetism. We report on the influence of spin polarized calculations on structure stabilization in bulk Co and Pt as well as the alloy*s various crystallographic phases: ordered L1o, L12, and disordered FCC. This approach corresponds to a quantitative first step towards better understanding the role of magnetism at the atomic scale.

Reference 1 (submitted): S. Karoui, H. Amara, F. Ducastelle, and B. Legrand, First principle study of order and magnetism in Co(1-x)Pt(x).

MM 33.5 Thu 12:45 IFW A

Finite temperature magnetism combining first-principles and spin Quantum Monte Carlo — •Fritz Körmann, Alexey Dick, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut Düsseldorf, Max-Planck-Straße 1, 40074 Düsseldorf

The free energy of a system is a fundamental quantity for predicting phase diagrams, finite temperature materials parameters, or kinetic barriers. An ab initio derivation of it makes a highly accurate evaluation of all excitation processes mandatory. One of the most challenging - but for many engineering materials crucial - contributions arises from the magnetic degrees of freedom. We have developed a mapping procedure that transforms the full magnetic Hamiltonian onto an effective nearest-neighbor spin Hamiltonian. The latter can be directly solved employing spin quantum Monte Carlo calculations. We demonstrate the high accuracy achievable by the new approach by computing magnetic heat capacities and free energies for the magnetic pure elements Fe, Co, and Ni, and by extending it to magnetic compounds such as Cementite (Fe3C) [1]. In all cases, an excellent agreement with experimental data is found.

[1] Hallstedt, Djurovic, von Appen, Dronskowski, Dick, Körmann, Hickel, Neugebauer, Calphad 34, 129 (2010).

MM 34: Nanomaterials I

Time: Thursday 11:00–13:00 Location: IFW B

MM 34.1 Thu 11:00 IFW B

Random structural inhomogeneities in the axial direction in high pressure torsion processed samples — •David Geist, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

High pressure torsion (HPT) is a widely used method of severe plastic deformation to produce bulk nanostructured materials. In this study, it is shown for the intermetallic compound Zr3Al by TEM and SEM methods that grain refinement happens in a random manner. This contradicts the commonly accepted HPT formula which predicts that grain refinement, prior to saturation, should have a radial dependence only. Unlike earlier findings of violations of the HPT formula, that showed systematic inhomogeneities along the axial direction due to material flow during the early stages of HPT deformation, this work presents a mostly random refinement behavior along both the radial and the axial direction. In this inhomogeneous structure, refined regions carry most of the deformation while coarse grained regions hardly get deformed. Local hardness measurements are able to explain this deformation behavior by revealing the refined structure being softer. To study in detail the interface regions between these structurally distinct sample volumes, some samples were surface treated prior to deformation, leading to a systematic localization of the refined regions at the sample surfaces. High resolution TEM of the interface region reveals twinned structures and high dislocation densities, that could arise by the large strain gradient present at the interfaces.

MM 34.2 Thu 11:15 IFW B

***In Situ* Probing of fast Defect Annealing in Cu and Ni with a High-Intensity Positron Beam** — •Bernd Oberdorfer[1], Eva-Maria Steyskal[1], Wolfgang Sprengel[1], Werner Puff[1], Philip Pikart[2], Christoph Hugenschmidt[2], Michael Zehetbauer[3], Reinhard Pippan[4], and Roland Würschum[1] — [1]Inst. f. Materialphysik, TU Graz (A) — [2]Physik Dept. E21 u. FRM II, TU München (D) — [3]Physik Nanostr. Mater., Fak. Physik, Univ.Wien (A) — [4]Erich Schmid Inst. Mater. Sci, Univ. Leoben (A)

The thermally activated annealing characteristics of atomic defects in ultrafine-grained, high purity Ni and Cu after severe plastic deformation (SPD) have been analyzed by means of positron annihilation techniques and dilatometry. This was realized using the high-intensity monoenergetic positron beam at the NEPOMUC positron source of FRM II which allows for fast, *in situ* temperature dependent positron-electron annihilation spectroscopy on a time scale of minutes. Furthermore, high-precision length change measurements with a difference dilatometer provided information about the amount of excess free volume in these SPD materials associated with defects such as vacancies, vacancy agglomerates, dislocations and grain boundaries. The combination of these two *in situ* methods, atomistic positron annihilation and macroscopic dilatometry allows for an identification of the structural defects in solids by means of a detailed analysis of their annealing kinetics upon linear heating [1]. Financial support by the Austrian Science Fund (FWF) is appreciated (project P21009-N20).
[1] B. Oberdorfer et al., Phys. Rev. Lett. **105**, 146101 (2010).

MM 34.3 Thu 11:30 IFW B

Grain boundary excess volume in metals determined by dilatometry — •Eva-Maria Steyskal[1], Bernd Oberdorfer[1], Wolfgang Sprengel[1], Michael Zehetbauer[2], Reinhard Pippan[3], and Roland Würschum[1] — [1]Inst. f. Materialphys., TU Graz, 8010 Graz, Austria — [2]Phys. Nanostrukt. Mater., Fakultät f. Phys., Uni. Wien, Austria — [3]Erich Schmid Institute of Mater. Sci., Leoben, Austria

The amount of excess volume in grain boundaries (GB) represents a physical key parameter which for instance determines the GB energy and GB diffusion. The direct method of time-differential dilatometry is applied in order to study the specific excess volume associated with grain boundaries by measuring the irreversible length change in submicrocrystalline (smc) Ni upon annealing-induced crystallite growth. In smc-Ni prepared by high-pressure torsion two annealing regimes occur of which the distinct stage at ca. 200°C is due crystal growth after structural relaxation. From the measured length decrease in this stage and the concomitant increase of the crystallite size as determined by scanning electron microscopy, an excess volume per unit area $\epsilon = (0.034 \pm 0.004)$ nm of relaxed grain boundaries is deduced. Taking into account the anisotropic grain structure, this value is independent of the measuring direction of the length change. The results will be compared with available literature data obtained from molecular dynamic simulations, high-resolution transmission electron microscopy, or indirect experimental techniques. Financial support by the FWF Austrian Science Fund is appreciated (project P21009-N20).

MM 34.4 Thu 11:45 IFW B

Grain boundary segregation of carbon and formation of nanocrystalline iron-carbon alloys by ball milling — •Yuzeng Chen, Andreas Herz, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Based on a novel defactants (defect acting agents) concept (R. Kirchheim, IJMR (Z. Metallkde) 100 (2009) 483 and Acta Materialia 55 (2007) 5129 and 5139), a novel method of understanding and synthesizing NC material was proposed by introducing defactants into materials to enhance the formation ability of nanocrystalline (NC) structures. Iron-carbon system was chosen as a model system where carbon acts as the so-called defactant. NC iron-carbon alloys with different carbon concentrations (C_0) were prepared by ball milling. Afterwards, the as-milled powder with relatively low carbon concentration was annealed at a certain temperature to achieve saturation of GBs by carbon. Mean grain sizes of the powders (D) were investigated by TEM and XRD. The results indicated that once the saturation of GBs is achieved, D will be strongly dependent on C_0 and will follow a mass balance of carbon in a closed system, i.e. $D = 3\Gamma_{gb}V_m/(C_0 - C_g)$ with C_g the carbon concentration in grains, Γ_{gb} the grain boundary excess, and V_m the molar volume. Based on the experimental results, the formation of NC iron-carbon alloys was treated within the framework of the defactant concept.

MM 34.5 Thu 12:00 IFW B

Laser radiation welding of transparent polymer foils by using noble metal nanoparticles as absorption layer — •Matthias Neuber, Thomas Hanke, Jörg Lucas, and Andreas Heilmann — Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Straße 1, Halle (Saale), Germany

Laser radiation welding of transparent polymer foils requires an additional absorption layer. Due to their optical plasmon resonance, metal nanoparticles can act as such an absorber. The spectral position, intensity and half width of the absorption peak are determined by the size and shape distribution of the particles as well as by the surrounding media. During carefully performed laser irradiation, the optical absorption behaviour of a thin nanoparticle layer is sufficient to join two much thicker transparent polymer foils and the particles change their size and shape basically by diffusion processes and melting processes of the polymer during this radiation process.

The metallic nanoparticles were deposited on the surface of ethylene tetrafluoroethylene foils by evaporation processes or magnetron sputtering. Laser irradiation was performed by a defocused continuous wave diode laser at a wavelength of 808 nm and a spot diameter of about 3 mm. During this radiation, the foils were welded and finally a nearly transparent welding seam was achieved. The nanostructures and the optical properties of the nanoparticle layers before and after laser irradiation were determined and compared. Mechanical tensile tests of the laser welding seams have demonstrated that their tensile strength is comparable to conventional thermal welding seams.

MM 34.6 Thu 12:15 IFW B

Ultrasound-driven design of new mesoporous metal catalysts — •Jana Schäferhans[1], Ekaterina Skorb[2], Nicolas Pazos Perez[1], and Daria Andreeva[1] — [1]Physikalische Chemie II, Uni Bayreuth, Deutschland — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Golm, Deutschland

Mesoporous metal nanocomposites were formed by a "green chemistry" method with ultrasound irradiation. The sonication technique combines the fabrication of a mesoporous support consisting of metallic particles (Al, Mg) several tens of micrometers in size and the subsequent incorporation of metal (Ag, Au, Pt etc.) nanoparticles into its pores. Next to filling the mesoporous support with particles we are

also able to form mesoporous alloys e.g. AlNi or CoAlFe. The resulting material is analyzed by transmission electron microscopy, powder X-ray diffraction, small-angle neutron scattering and the Brunauer-Emmett-Teller and the Barrett-Joyner-Halenda method. Surface areas up to 200 m^2/g with a narrow pore size distribution around 3 nm can be achieved. The mesoporous structures are analyzed by confocal light microscopy after coloring the particles with dye. We explain the formation of the mesoporous inner structures by the following mechanism: Thermal etching and recrystallization of metals by ultrasound-stimulated high-speed jets of liquid form the porous structure that is stabilized by surface oxidation through free radicals generated during cavitation. We expect this approach to be universal and opening perspectives for a whole new class of catalytic materials that can be prepared in a fairly easy and cost effective way.

MM 34.7 Thu 12:30 IFW B

Correlation of structure and electron transport in Fe filled carbon nanotubes — •Vadim Migunov, Marina Spasova, and Michael Farle — Fakultät für Physik, and CeNIDE University Duisburg-Essen, 47048 Duisburg, Germany

Carbon nanotubes (CNT) are potentially the interesting building blocks for different types of future electronic and mechanical devices. The filling of CNT with magnetic materials opens new multifunctional possibilities for novel applications.

The Fe filled CNT (FeCNT) were synthesized by chemical vapor deposition [1]. Transport studies were conducted inside a Philips CM-12 transmission electron microscope (TEM) using Nanofactory scanning probe microscopy (SPM) holder for TEM. A gold SPM tip was brought in contact with a single FeCNT, and two-point resistance measurements were carried out.

We have found that high current densities ($>10^{10}$ A/m^2) lead to evaporation of Fe in FeCNT. After the evaporation the total resistance of the system decreases by up to a factor of three as confirmed by steps in the I-V curves.

The work has been supported by SFB 445. The FeCNT were prepared by the CVD group of the IFW Dresden.

[1] A. Leonhardt, M. Ritschel, R. Kozhuharova, A. Graff, T. Muhl, R. Huhle, I. Monch, D. Elefant, C. M. Schneider, Diamond and Relat. Mater. 12, 790 (2003)

MM 34.8 Thu 12:45 IFW B

Electrical properties of an Al-NWFET fabricated under different gate oxide layers — •Dawit Gedamu[1], Torge Behrendt[1], Hermann Kohlstedt[2], Ondrej Vavra[2], Adrian Petraru[2], and Rainer Adelung[1] — [1]Functional Nanomaterials, Institute of Materials Science, Faculty of Engineering, University of Kiel, Kaiser Strasse 2, 24143 Kiel, Germany — [2]Nanoelektronik, Technische Fakultät Kiel, Christian-Albrechts-Universität Kiel, 24143 Kiel , Germany

Recently 1 D nanostructures such as nanowires (NWs) becoming gradually more important as components for micro- and nanoelectronic devices because of their high surface to volume ratio [MRS Bulletin 32, 99 (2007), Acc. Chem. Res. 32, 435 (1999)]. Nonetheless, the development of 1D NWs with desired thicknesses on preferred substrates or between two metal contacts as well as their understanding their physical properties, are the still challenging. Several methods have been utilized so far to grow 1D NWs but according to industrial demand, we have used thin film fracture [Nat. Mater. 3, 375 (2004)] as NW templates and electron beam lithography techniques to fabricate Al NW field effect transistors (NWFETs). The fabrication of Aluminum NWFETs with dimensions in the sub-100 nm regime and the electrical characteristics of bottom gate FETs will be presented. An 100 nm thick silicon dioxide on 380 micron thick <100> oriented p-doped silicon was used gate oxide. In another approach, Alumina film synthesized through electrochemical oxidation on silicate glass substrate was used to as gate dielectric. A close analysis of the NWFETs reveals a slight drop down of the conductance with increasing gate voltage.

MM 35: Topical Session Heterogeneous Nucleation I

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

Topical Talk MM 35.1 Thu 11:00 IFW D

On selected methodological challenges at the interface between quantum-mechanical approaches and phase-field modeling methods in computational materials science — •Martin Friak[1], Li-Fang Zhu[1], Alexey Dick[1], Alexander Udyansky[1], Johann von Pezold[1], Heike Emmerich[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Universität Bayreuth, Bayreuth, Germany

In order to reliably describe complex materials-science phenomena that are often bridging multiple length and time scales, different methods must be effectively combined. Achieving a seamless methodological interface between fundamentally different approaches still presents a major challenge despite of systematic and long-standing efforts. For the theoretical study of microstructural processes in multi-component and multi-phase metallic alloys considered here, a combination of quantum mechanical calculations and phase-field modeling constitutes the method of choice. In particular, the transferrability of quantum mechanical calculations ensures the predictive power of the approach, while the phase field model extends the accessible length and time scales in our simulations. The talk will critically review selected problems arising when ab initio calculations and/or atomistic simulations are employed to parametrise phase-field models for (i) the evaluation of the temperature dependence of thermodynamic, structural and elastic properties of different phases, (ii) the prediction of diffusion parameters, as well as (iii) the description of solid/liquid and solid/liquid interfaces.

MM 35.2 Thu 11:30 IFW D

Scale-Bridging Simulation on Atomistic and Mesoscopic Length Scales. — •Marco Berghoff[1] and Britta Nestler[1,2] — [1]Institute of Materials and Processes, Hochschule Karlsruhe, Germany — [2]Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology (KIT), Germany

In the present analysis we study the process of early stage solidification using molecular dynamics (MD), phase-field crystal (PFC) and the phase-field (PF) methods. While the MD and the PFC methods are mostly in use at the atomistic scale, the PF can make meaningful predictions at the mesoscale. To demonstrate the ability of the PF in applications at the atomistic scale, we conduct a comparative study of growth of pure Ni in the early stage of solidification between MD and PF simulations. For this, the discrete atomic positions from the MD simulations are converted to a continuous field of the PF order parameter differentiating the phases, using the q_6q_6 operation. In addition, we tailor the parameters in the PF model to match those used in the MD model with a temperature dependent specific heat capacity and latent heat. We then compare the volume change of the nucleus as a function of time occurring in both simulation methods. As a substitute to MD simulations, we also used the PFC method for generating data at the atomistic scale, and compared the results with PF simulations. The ultimate goal is to benchmark the atomistic simulations with the PF method at the smaller scale and thereafter conduct PF simulations at the mesoscale, which is outside the realm of atomistic simulation methods.

MM 35.3 Thu 11:45 IFW D

Crystal growth, solid-liquid interfaces and nucleation in simple model systems: Computer simulations of Nickel — Roberto E. Rozas and •Jürgen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Molecular dynamics as well as Monte Carlo simulation techniques are used to investigate crystal growth, solid-liquid interfaces and nucleation in Nickel. To determine various interfacial properties, inhomogeneous systems are prepared where the crystal phase at different orientations coexists with the fluid phase, separated by planar interfaces. Interfacial stiffness and tension are estimated using different predictions of capillary wave theory with respect to the capillary wave spectrum, finite-size broadening of the interfacial width and different geometries of the interface. Free energy barriers for the formation of a nucleus from the melt are computed via Monte Carlo simulation in conjunction with umbrella sampling techniques. Good agreement with recent experiments on Ni is obtained.

MM 35.4 Thu 12:00 IFW D

Phase-field simulations of inoculation and subsequent peritectic solidification in Ti-Al-B — •Markus Apel, Janin Eiken, and Ulrike Hecht — Access, RWTH Aachen

In Ti-Al based alloys boride particles can be used as grain refiners. By varying the B content in the melt, the formation temperature of boride particles can be adjusted in a way that they act as heterogenous nucleation sites for either the properitectic β- or the peritectic α-phase. We elucidate the effect of borides on microstructure formation by phase-field simulations coupled to a thermodynamic database. Nucleation and growth of small boride particles are explicitly taken into account on a scale below the numerical phase-field interface thickness by using a semi-analytical growth model. The simulation results show a variety of effects: grain refinement due to heterogeneous nucleation on TiB2-particles, interactions between the growing Ti phases and the borides, as well as a pronounced dependency of the phase transformation rates on the dominant nucleation sites.

MM 35.5 Thu 12:15 IFW D

growth of a two-phase finger in eutectic systems — •Guillaume Boussinot[1,2], Claas Hueter[1,2], and Efim Brener[1] — [1]forschungszentrum juelich — [2]MPIE duesseldorf

We present a theoretical study of the growth of a two-phase finger in eutectic systems. This pattern was observed experimentally by Akamatsu et al., Phys. Rev. E 61, 3757 (2000). We study this two-phase finger using a boundary-integral formulation and we complement our investigation by a phase-field validation of the stability of the pattern. The deviation from the eutectic temperature and from the eutectic concentration provide two independent control parameters, leading to very different patterns depending on their relative importance. We propose scaling laws for the velocity and the different length scales of the pattern.

MM 35.6 Thu 12:30 IFW D

Dendritic solidification along liquid-liquid interfaces — •Claas Hüter[1,2], Guillaume Boussinot[1,2], Efim Brener[2], Dimitri Temkin[2], and Robert Spatschek[2] — [1]MPIE, Düsseldorf — [2]Forschungszentrum Jülich

Solidification of an asymmetric dendrite along the interface of two liquids is discussed. The considered system shows a monotectic reaction, the diffusion equations and the associated thermodynamic boundary conditions are represented by three coupled nonlinear integral equations. The selection in this case determines the velocity, the lengthscale of the parabolic asymptotics of the dendrite and the lengthscale which defines the liquid-liquid interface. These quantities are determined as functions of the undercooling numerically.

MM 35.7 Thu 12:45 IFW D

Experimental determination of nucleation rates — •Joachim Bokeloh and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Upon cooling a metallic melt, the nucleation rate changes from practically zero to virtually infinite in the small range of accessible crystallization temperatures, thus leaving only a narrow temperature window for experimental as well as for computational investigations. Both, the system size and the time scale of computational studies differ from those within reach of experimental studies by several orders of magnitude. Thus, for a meaningful comparison of computational and experimental works, the nucleation rates have to be extrapolated over several orders of magnitude. For this procedure, an accurate coverage of the nucleation rate over the complete accessible range is imperative. We present here data on the liquid undercooling behavior of Nickel obtained by repeated melting and crystallization in a DTA. This method allows acquiring a statistically meaningful data set under clean and reproducible conditions, from which nucleation rates can be determined. Supported by a variation of the sample mass from 10μg to 60 mg and classical isothermal nucleation rate measurements, the nucleation rate of pure Nickel was determined experimentally over a range of eight orders of magnitude and a temperature window of 70 K, thus allowing a true quantitative testing of the classical nucleation theory. Nickel was chosen as a model system because it shows high levels of undercooling and a well refined embedded atom potential is available for concurrent simulations.

MM 36: Topical Session Electron Theory V

Time: Thursday 14:00–16:00 Location: IFW A

Topical Talk MM 36.1 Thu 14:00 IFW A

Thermodynamics and Kinetics of Grain Boundary Junctions — •Guenter Gottstein, Luis Barrales, Lasar S. Shvindlerman, and Bingbing Zhao — RWTH Aachen University, Institute of Physical Metallurgy and Metal Physics, 52056 Aachen, Germany

Grain Boundaries in polycrystals are connected by grain boundary junctions, which coordinate the kinetic behavior of grain boundary systems, like migration or segregation. Therefore, grain boundary networks are likely to behave differently from solitary grain boundaries. We show that grain boundary junctions are crystal defects on their own with specific thermodynamic and kinetic properties and that these properties affect microstructural evolution during grain growth. Novel experimental methods will be introduced on how to determine the thermodynamic and kinetic properties of junctions, and theoretical approaches will be proposed how to modify existing theories of polycrystal kinetics to account for junction effects. Finally, computer simulations of grain boundary motion and grain growth will be presented to demonstrate the effect of junctions on kinetics, grain size, and texture.

Topical Talk MM 36.2 Thu 14:30 IFW A

High-performance permanent magnets - significance of thermodynamics, kinetics and microstructure — •Gerhard Schneider and Dagmar Goll — Aalen University, Materials Research Institute, Beethovenstr. 1, 73430 Aalen

High-performance permanent magnets (pms) like NdFeB magnets are based on outstanding intrinsic and extrinsic (microstructural) magnetic properties. Excellent intrinsic properties as high saturation polarization and large magnetic anisotropy are achieved by combining transition-metal atoms and rare-earth atoms. For outstanding extrinsic properties ideally μm- or nm-scaled textured hard magnetic grains of ellipsoidal shape are required separated by a nonmagnetic grain boundary phase from each other. However, in NdFeB sintered pms deviations ("structural defects") from this ideal microstructure occur due to the chosen alloy composition in the phase diagram (including additives), powder processing, sintering and annealing conditions. As a consequence the microstructure is characterized by hard magnetic grains of polyhedral shape which are completely or partly surrounded by grain boundary phases (metastable magnetic phases, nonmagnetic phases (η-phase, rare earth oxides)) and pores. Especially the metastable phases which crystallize out of a liquid phase at sintering form a complex structure below the eutectic solidification temperature of 650 °C and influence the magnetic properties. The presentation highlights the thermodynamics and kinetics of the grain boundary phases. The systematic quantitative investigation of character and composition of these phases enables a specific tailoring of the properties of high-performance pms.

MM 36.3 Thu 15:00 IFW A

Thermodynamic model of alloy grain boundaries — •Alexander Kirchner — Institut für Werkstoffwissenschaft, Technische Universität, 01062 Dresden, Germany

A facile thermodynamic model for grain boundaries in substitutional alloys is developed. The macroscopic analysis is based on established descriptions of metallic solutions and the universal equation of state at negative pressure. The thermodynamic potential free energy of atoms in grain boundaries is derived as a function of excess volume and composition. Employing Guggenheim's condition for equilibrium between bulk phase and grain boundaries, the interface free energy and segregation enrichment are expressed. For binary systems with known segregation behavior these quantities are calculated. The results show good agreement with experimental data. Despite inherent limitation which are discussed the proposed model is especially useful for the understanding of nanocrystalline materials.

MM 36.4 Thu 15:15 IFW A

Ab initio prediction of thermodynamic data for selected phases of the Al-Mg-Si-Cu system — •Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Joerg Neugebauer — Max-Planck Institut fuer Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Duesseldorf, Germany

Al-Mg-Si-Cu alloys are widely used in engineering applications due to their excellent mechanical properties: low density, high hardness and melting temperature. To tailor these properties, quantitative simulations (like CALPHAD) rely on exact thermodynamic potentials which are nowadays mostly derived from calorimetric experiments. First principles calculations emerge as an alternative for reliable thermodynamic functions in cases of non-existent experimental data or in regions of phase boundaries where the reliability of experiments is limited due to the transient nature of metastable phases. We have, therefore, calculated highly accurate ab initio free energies as a function of temperature and molar volume for selected binary, ternary and quaternary phases of the Al-Mg-Si-Cu system with focus on hcp Mg, diamond Si and Mg2Si. Various quantities are derived from the thermodynamic potentials: Gibbs free energies of formation, enthalpies, entropies, heat capacities, thermal expansions, vacancy concentrations etc. We compare our results to a variety of experiments and put special emphasis on temperature effects due to lattice vibrations. We find the Debye model not to be sufficient at high temperatures and demonstrate that our consistent ab initio approach can improve previous CALPHAD parameterizations of Mg2Si with respect to current experiments.

MM 36.5 Thu 15:30 IFW A

Non-scalar cluster expansions for arbitrary configuration dependent observables in advanced materials — •Sascha B. Maisel[1], Nils Schindzielorz[1], Karsten Durst[2], and Stefan Müller[1] — [1]Hamburg University of Technology, Institute of Advanced Ceramics, Denickestrasse 15, 21073 Hamburg, Germany — [2]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Werkstoffwissenschaften, Martensstrasse 5, 91056 Erlangen, Germany

We use DFT-based approaches to calculate both free energies and various quantities of technological relevance. These include bulk moduli, elastic constants, piezo-response tensors and dielectric constants of high-end materials like Ni-rich alloys and lead-free ferroelectrics. Based on the formalism of the cluster expansion [1] as realized in the UNCLE [2] package, it is possible to expand any configuration dependent observable like the formation enthalpy in terms of its many-body interactions. In this talk, we present several cluster expansions performed for multiple observables simultaneously. These types of cluster expansion each yield the formation enthalpy plus one or more of the aforementioned other quantities. This enables us to relate e.g an elastic constant of a structure with its chemical stability.

[1] J. M. Sanchez, F. Ducastelle, D. Gratias: Physica 128 A, 334, (1984)

[2] D. Lerch, O. Wieckhorst, G. L. W. Hart, R. Forcade, S. Müller: Modelling Simul. Mater. Sci. Eng. 17, 055003, (2009)

MM 36.6 Thu 15:45 IFW A

Temperature dependence of the stacking fault energy in $Fe_{0.716}Cr_{0.200}Ni_{0.084}$ alloy from first principles — •Hojjat Gholizadeh[1,2], Andrei Reyes-Huamantinco[1,2], Andrei Ruban[3], Peter Puschnig[1], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Austria — [3]Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden

The mechanism of plastic deformation of steels under mechanical stress is governed by the magnitude of the stacking fault energy (SFE). We calculate the SFE for $Fe_{0.716}Cr_{0.200}Ni_{0.084}$ random alloy in paramagnetic austenitic phase in the temperature range 300-1500 K. Our methodology uses the axial interaction (ANNNI) model to calculate the SFE as a function of the free energies of the perfect fcc, hcp, and double-hcp crystal phases. These free energies are dependent on the lattice parameter which is obtained from experimental thermal expansion data, and on the local magnetic moments which are evaluated using DFT calculations and a Monte-Carlo simulation of a magnetic Hamiltonian of independent local moments. The DFT calculations are performed using the exact muffin-tin orbitals (EMTO) method, which enables to use the coherent potential approximation (CPA) and the disordered local moment (DLM) approaches to model the random alloy in paramagnetic state. Our results, in particular the SFE(T=300 K)=15 mJ/m^2 and the hcp↔fcc transition temperature of 550 K, are in good agreement with experiments.

MM 37: Nanomaterials II

Time: Thursday 14:00–16:00 Location: IFW B

MM 37.1 Thu 14:00 IFW B

graphene, magnetism, hubbard, — •Jin-Jun Liang and Ping Huai — Shanghai Institute of Applied Physics, Shanghai, China

We investigate magnetic properties of defective graphene, using a modified Hubbard model of the pi electrons of the carbon atoms. Spin interaction between pi elections and dangling sp2 bond has been taken into consideration. Mean field approximation is employed in our calculation, in order to deal with very large fragment of graphene. Magnetism of graphene with different types of defects will be presented in this talk.

MM 37.2 Thu 14:15 IFW B

Metallic nanowire growth from solution using dielectrophoresis — •Alexander Nerowski[1], Markus Poetschke[2], Manfred Bobeth[2], Walter Weber[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01069 Dresden, Germany — [2]Institute for Materials Science, Dresden University of Technology, 01069 Dresden, Germany — [3]NamLab gGmbH, 01187 Dresden, Germany

A lot of effort has been made to manufacture metallic nanowires by top-down procedures as classical lithography. Metallic nanowire growth from solution represents a promising inexpensive bottom-up method working at room temperature. By applying an AC voltage, nanowires grow on a substrate between two electrodes in a solution containing metal complexes. Aiming at a controlled growth of straight and as thin as possible wires, the growth process is investigated both experimentally and theoretically. The nanowire itself, since it is conductive, is modeled as a half-sphere electrode. Our model includes the dielectrophoretic force on uncharged metal complexes as well as their diffusion in the solution. In particular, the growth velocity of the wire is found to depend only weakly on the applied voltage since the overall growth process is diffusion-controlled. Difficulties in comparing theoretical predictions and experimental observations due to poorly known material parameters are discussed. For reasonable parameter choices, the calculated nanowire growth velocity is in modest agreement with measurements.

MM 37.3 Thu 14:30 IFW B

Synthesis and characterization of Tin Oxide nanowires and nanobelts — •Ingo Paulowicz, Yogendra Kumar Mishra, Arnim Schuchardt, Viktor Hrkac, Lorenz Kienle, and Rainer Adelung — Christian Albrechts Universität Kiel, Technische Fakultät, Kaiserstraße 2, 24143 Kiel, Deutschland

Recent developments in the direction of semiconducting oxide nanostructures have provided new dimensions in energy harvesting and storage, battery materials, solar cells, flat panel displays and others in terms of miniaturization, response and cost effectiveness [1]. Beside zinc oxide, tin oxide is the second most important member in the class of metal oxide semiconductors. It is currently undergoing different processes of synthesis to produce cost effective electronics and other devices. Several complicated synthesis methods, starting from vapor liquid solid, have been used to synthesize 1-D nanostructures of tin oxide. In present work we report a very simple flame assisted versatile and cost effective technique for growing SnO2 nanorods, nanowires, nanobelts and their networks with macroscopic expansion on the cm scale. Growth and crystalline nature of nanorods were investigated by high resolution transmission electron microscopy, which revealed [100] and [101] growth and twin boundary propagation. Mechanical properties of tin oxide nanobelts and electrical properties of nanorods will be discussed.

Z. L. Wang et al., Adv. Mater. 15, 432 (2003), Annu. Rev. Phys. Chem. 55, 159 (2004).

MM 37.4 Thu 14:45 IFW B

Boron nanotubes: new players on the nano-field — •Viktor Bezugly, Jens Kunstmann, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01069 Dresden, Germany

The existence of pure boron nanotubes (BNTs) has been proposed more than ten years ago [1]. The BNTs are predicted to have a metallic conductivity independent of their diameter and chiral angle [1-3], in contrast to the well-studied carbon nanotubes. This property makes BNTs good candidates for nanometer-scale conducting elements of future electronic devices. Recent experimental work on BNTs [4] has provided the first evidence for their metallic behavior. Nevertheless, there are still many open questions on the physical properties of BNTs which need to be answered on both the theoretical and experimental sides. In our work we theoretically investigate the electronic structure and transport properties of large-diameter BNTs of different structures and chiralities. Our results are in agreement with recent experimental findings, and a method to control the electron transport in BNTs is proposed.

References: [1] I. Boustani, A. Quandt, E. Hernandez, A. Rubio, J. Chem. Phys. 110, 3176 (1999); [2] J. Kunstmann, A. Quandt, Phys. Rev. B 74, 035413 (2006); [3] N.G. Szwacki, C.J. Tymczak, Chem. Phys. Lett. 494, 80 (2010); [4] F. Liu, C. Shen, Z. Su, X. Ding, S. Deng, J. Chen, N. Xu, H. Gao, J. Mater. Chem. 20, 2197 (2010).

MM 37.5 Thu 15:00 IFW B

Charging Gold Nanoclusters in Ionic Liquids — •Alexander Held and Michael Walter — FMF Uni Freiburg, Germany

Structures at the nanometer scale show quantized charging effects that can be observed by differential pulse voltammetry experiments. The charge dependent cluster capacitance of gold nanoclusters in the ionic liquid BMImBF4 is investigated using density functional theory (DFT) simulations. The DFT results can be understood via a semiclassical model describing the effect of a polarity inversion of the BMImBF4 double layer on the charge dependent cluster capacitance. These models also explain features seen in recent experimental data.

The DFT calculations have been carried out using the state of the art projector augmented wave method on a real space grid with the GPAW [1] implementation.

[1] https://wiki.fysik.dtu.dk/gpaw/

MM 37.6 Thu 15:15 IFW B

Atomistic simulations of nano-scale impact on phonon modes of Ge — •Daniel Sopu[1], Jani Kotakoski[2], and Karsten Albe[1] — [1]Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]Division of Materials Physics, University of Helsinki, P.O.Box 42, 00014 Helsinki, Finland

Using molecular dynamic simulations, we have studied the phonon density of states of different nano-structures like nanoparticles, nanocrystals, embedded nanoparticles and nanoglasses. We investigate the vibrational properties of Germanium as an example for a covalently bonded material using two different interatomic potentials. By comparing the vibrational properties of the nanostructures to single crystalline and bulk amorphous structures, significant deviations have been found. For each structure individually, the predominating finite-size effect was identified. We developed a complete description of size effects on phonon density of states in terms of disorder, phonon confinement due to the particle, and surface stress.

MM 37.7 Thu 15:30 IFW B

Molecular dynamics study of diffusion-induced recrystallisation — •Sebastian Manuel Eich, Michael Kasprzak, and Guido Schmitz — Institute of Material Physics, University of Muenster, Germany

Diffusion-induced recrystallisation (DIR) was investigated in thin film Au-Cu and Ni-Pd interdiffusion couples. Characteristic concentration levels are observed inside newly formed grains instead of the expected continuous Ficks diffusion profiles. This effect seems to be related to elastic mismatch strain in the diffusion zone. Experimental results reveal a relationship between characteristic compositions and the ideal shear strength of metals. Within the diffusion zone, the characteristic compositions are always adjusted so that a maximum stress of about 70% of the ideal shear strength is established. In our model, we use molecular dynamics based on embedded-atom potentials (EAM) to study the process of DIR in gold-copper diffusion couples. We simulate the stress development in thin (3-6 nm) copper layers fixed to a substrate. Step by step, copper atoms are replaced by gold. We observe a linear increase in stress with gold concentration until a critical level is reached and spontaneous relaxation and break of coherency take place. Using different conditions (temperature, external pressure ...), we are able to confirm that the maximum stress is close to, but always lower than the ideal shear strength in the dominant slip system.

MM 37.8 Thu 15:45 IFW B

High-temperature thermal stability of nanocrystalline iron — •Jules M. Dake and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Nanocrystalline materials promise enhanced properties, but the realization and application of such materials is limited by their thermal stability. The large specific grain-boundary area leads to a strong driving force for grain growth, which can, in some cases, occur at or even below room temperature [1]. When atoms of a second species with an appreciable segregation enthalpy are introduced, they should, in theory, reduce the grain-boundary energy and thus the driving force. Exactly this has been reported for numerous binary systems, as summarized in [2]. Our investigations of binary Fe alloys show similar results up to a temperature of $\sim 900°C$. Above this limit, however, stability is suddenly lost. *In situ* XRD results appear to incriminate the α-to-γ transformation. Direct observation of the microstructure by FIB microscopy reveals a growth morphology similar to that of recrystallization or abnormal grain growth.

[1] M. Ames *et al.*, *Acta Mater.* **56** (2008) 4255–4266.
[2] J. R. Trelewicz and C. A. Schuh, *Phys. Rev. B* **79** (2009) 094112.

MM 38: Topical Session Diffussionless Transformations I

Time: Thursday 14:00–16:00 Location: IFW D

Topical Talk MM 38.1 Thu 14:00 IFW D

Epitaxial films of the magnetic shape memory alloy Ni2MnGa — •Gerhard Jakob, Tobias Eichhorn, Richard Hausmanns, Peter Klaer, Michael Kallmayer, and Hans-Joachim Elmers — Institute of Physics, Johannes Gutenberg-University Mainz

While large magnetically induced strains up to 10% have been observed for bulk single crystals of Ni_2MnGa, these large effects have not been demonstrated for thin films of this compound yet. The preparation of free standing single crystalline films turns out to be a challenging task, but is a necessary precondition for applications on smallest scale.
We report on the preparation and investigation of thin epitaxial films of the NiMnGa-system via dc-magnetron sputtering from an alloy target to heated substrates as Al2O3(11-20), MgO(100) and NaCl(100). The complex crystal structure is studied by temperature dependent x-ray diffraction in 4-circle geometry, whereas magnetic properties are investigated by magnetometry. To avoid blocking effects of the substrate free standing films were prepared by introduction of a buffer layer on MgO(100) that can be etched away selectively.
Using X-ray absorption spectroscopy we determined the element specific magnetic moments and found a remarkable change of the Ni X-ray absorption spectra occurring at the temperature of the phase transition (Tm) which indicates specific changes of the electronic structure. The observed changes are in agreement with theoretical predictions.
This work is part of the DFG priority program SPP 1239.

MM 38.2 Thu 14:30 IFW D

Transition from modulated to non-modulated martensite in thin Ni-Mn-Ga films — •Anja Backen[1,2], Bernhard Holzapfel[1], 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, Department of Mechanical Engineering, Institute of Materials Science, 01062 Dresden, Germany

In Ni-Mn-Ga, an external magnetic field can induce strains of up to 10% by twin boundary motion. One condition for this MSM effect is a twinning stress of 2 MPa or less, which only the modulated martensite fulfills. The coexistence of 14-layer modulated (14M), non-modulated martensite (NM) and austenite in epitaxial films make them a model system to study the transition between the different martensitic phases. Kaufmann et al. [PRL 104 (2010) 145702] recently showed that 14M can be described as nanotwinned NM which forms at the austenite-martensite interface reducing elastic energy for the cost of twin boundary energy. With increasing distance to the interface, the elastic energy becomes less important and 14M transfers to NM by coarsening. To probe this, we examined Ni-Mn-Ga films of varying thickness deposited on MgO(100) substrates with a Cr buffer layer. Taking the integrated XRD-intensity ratio as a measure of phase fraction, we observe an increase of NM with increasing film thickness up to a maximum value of 63%. We conclude that for films on rigid substrates coarsening is inhibited by the elastic energy at the interface for one third of all possible 14M variants. This work is funded by DFG via SPP 1239.

MM 38.3 Thu 14:45 IFW D

Correlating twinning periodicity and film thickness of epitaxial Ni-Mn-Ga films — •Anett Diestel[1,2], Anja Backen[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, Department of Mechanical Engineering, Institute of Materials Science, 01062 Dresden, Germany

In order to probe the theoretical geometrical theory by Kiselev et al. [1] about the periodicity of stripe domains in magnetic shape memory alloys, we have analysed the finely twinned microstructure of 14M martensite in epitaxial Ni-Mn-Ga films. Epitaxial Ni-Mn-Ga films with different thicknesses ranging from 30 nm to 2 μm have been deposited by sputter deposition on single crystalline MgO(100) substrates with a chromium buffer layer. The characteristic microstructure of 14M martensite was quantified by atomic force microscopy. The periodic height profiles of the mesoscopic twin boundary formation were analysed according to the geometrical model of a twinned surface by Buschbeck et al. [2]. We observed an increasing twin boundary periodicity with the square root of the film thickness. We did not observe the increase of variant size below a critical thickness predicted by Kiselev et al. We attribute this to the finite number of unit cells involved, an aspect not considered in continuum theory. This work was funded by DFG through SPP 1239. [1] N.S. Kiselev et al. Eur. Phys. J. Special Topics 158 (2008) 119 [2] J. Buschbeck et al. Acta Mater. 57 (2009) 2516

MM 38.4 Thu 15:00 IFW D

Modelling Bain path and adaptive martensite in Fe-based magnetic shape memory alloys — •Markus Ernst Gruner[1], Sandra Weiss[2], Sebastian Fähler[2], Ludwig Schultz[2], and Peter Entel[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden

Magnetic shape memory (MSM) exhibit macroscopic strains of several percent in realistic magnetic fields. Apart from the prototypical system Ni-Mn-Ga also Fe-based alloys as fct $Fe_{70}Pd_{30}$ are considered for technological applications. Within this contribution we investigate the ground state behavior and finite temperature magnetism of MSM Fe-Pd alloys by means of large scale density functional theory calculations with up to 500 atoms including atomic relaxations, which are essential for an accurate description of structural properties [1]. On the essentially flat binding surface the ground state is found to be bct, while for tetragonal distortions beyond fcc an adaptive structure consisting of bct building blocks effectively decreases the energy. Also, magnetic excitations are capable of substantially altering the binding surface. The results agree closely with experimental evidence obtained from strained Fe-Pd MSM alloys epitaxially grown on different substrates, which cover the Bain path [2] and beyond confirming that adaptive structures can be deliberately grown in Fe-based MSM films.

This work is supported by the DFG through SPP 1239 and the supercomputing resources of the NIC, FZ Jülich.

[1] M. E. Gruner, MRS Symp. Proc. **1200E**, 1200-G04-04 (2010)
[2] J. Buschbeck *et al.*, Phys. Rev. Lett. **103**, 216101 (2009)

MM 38.5 Thu 15:15 IFW D

Probing the electronic origin of a martensitic transformation in frozen intermediate stages. — •X. Kozina[1], S. Weiss[2], L. Schultz[2], S. Fähler[2], G. Stryganyuk[1], S. Ouardi[1], G. H. Fecher[1], C. Felser[1], S. Ueda[3], and K. Kobayashi[3] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]IFW Dresden, Germany — [3]National Institute for Materials Science, SPring-8, Hyogo, Japan

An energetically unfavourable high density of states close to Fermi level had been suggested as driving force for martensitic transformation in metals. Here we present a direct experimental proof for the $Fe_{70}Pd_{30}$ magnetic shape memory alloy. By coherent epitaxial film growth we stabilize intermediate stages along the Bain transformation path, connecting *bcc* and *fcc* structure. This allows a detailed analysis at a constant temperature of 300 K, in vicinity of the martensitic transformation temperature. For probing the electronic structure of these 50 nm-thick films hard X-ray photoelectron spectroscopy (HAXPES) at BL15XU at SPring-8 was used. High probing depth of this method makes it a unique, non-destructive tool for studying electronic properties of thin films without taking into account the quality of the surface. Further, at high excitation energies one reaches nearly equal spectral weight for all states. Our measurements reveal that the density of states at 2 eV below the Fermi energy is reduced by 4,6% when the structure changes from the *fcc* austenite towards the *bcc* martensite. This confirms the proposed band Jahn Teller effect. *This work is supported by DFG through SPP 1239 and DfG-JST (FE633/6-1).*

Topical Talk MM 38.6 Thu 15:30 IFW D

Phase Transformations in Bi-based lead-free piezoceramics — •Jürgen Rödel and Wook Jo — Institute of Materials Science, Technische Universität Darmstadt,, Darmstadt, Germany

Piezoceramics in the application as an actuator experience electric fields between 0 and 3 kV/mm and temperatures between -30°C and 150°C with uniaxial stress up to 40 MPa. Lead-containing materials have relied on the concept of a morphotropic phase boundary (MPB), where similar free energy functions between rhombohedral and tetragonal afford easy polarization rotation and domain switching.

In this talk, the focus will be placed on the main lead-free piezoceramic material with MPB. Bismuth-Natrium-Niobate (BNT) - Barium titanate (BT)exhibits a pseudocubic structure at the MPB, which transforms irreversibly into a mixture of tetragonal and rhombohedral phases upon poling. this transformation, however, is reversible, if small amounts of Niobates are added. This leads to a very field-induced strain (poling strain+unipolar strain). the phase transition behavior will be presented utilizing in-situ (under electric field) investigations under synchrotron diffraction, neutron diffraction and in the TEM. Further, first diffuse scattering measurements on single crystals will be presented. Some of these measurements have been performed as function of temperature and are always discussed with respect to salient electrical performance.

MM 39: Computational Materials Modelling V

Time: Thursday 16:15–19:00 Location: IFW A

MM 39.1 Thu 16:15 IFW A

First-principles phase stability calculations of $Al_3(Ti_{1-x}Nb_x)$ pseudobinary alloys — •Yuhong Liu[1,2], Peter Puschnig[1], Ernst Gamsjäger[2], and Claudia Ambrosch-draxl[1] — [1]Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Institute of Mechanics, University of Leoben, Austria

In the TiAlNb-system(mole fraction of Al amounts to 0.75), the intermetallic ε-phase can exist in the $L1_2$, $D0_{22}$, or $D0_{23}$ structure. Experimental results indicate that the addition of Nb shows a site preference for the Ti sublattice. Therefore, we calculate the thermodynamic properties of $Al_3(Ti_{1-x}Nb_x)$ by assuming a pseudo-binary alloy system. We utilize the ATAT package to perform the sublattice cluster-expansion approach. Total energies of various ordered supercell structures are obtained within density-functional theory using the projector augmented wave (PAW) method as implemented in the VASP code. Effective cluster interactions derived from the structure-inversion method are then used in an Ising-type Hamiltonian, which

is solved by Monte-Carlo simulations. Our results show that the addition of Nb stabilizes the cubic $L1_2$ structure relative to the $D0_{22}$ and $D0_{23}$ ones. We find the effect of short-range-order on the calculated formation energies to be small compared to random mixing on the Ti-Nb sublattice. At high temperature, thermodynamic quantities such as the enthalpy and free energy are extracted from the Monte-Carlo simulations and compared to results from the CALPHAD method.

MM 39.2 Thu 16:30 IFW A

Hydrogen solution enthalpies derived from first principles: Chemical trends along the series of transition metals — •Ugur Aydin[1], Sixten Boeck[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung — [2]Gemmantics IT-Consulting

Since the mid-19th century it has been known that some transition metals (TM) can absorb significant amounts of hydrogen, whereas others cannot. Since the presence of this interstitial atom can lead to serious materials failures, the energetics and dynamics of hydrogen in TMs are of critical importance in state-of-the-art materials design. Most of the previous studies, considering the hydrogen solubility for a larger number of TMs, rely on experimental observations and/or semi-empirical models. However, the ability of these models to provide a deeper understanding and insight into the decisive underlying mechanisms involved in hydrogen-solubility is limited. In our work, we therefore employed ab initio calculations to systematically investigate the mechanical and chemical mechanisms governing hydrogen solution in a complete set of TM under comparable conditions. The solution enthalpy for H in the high symmetry interstitial sites of TMs has been calculated consistently assuming various crystallographic / magnetic structures. For the data management a sophisticated automatic database has been developed. The analysis of this complete set of data allowed us to detect an universal dependence of the H solution enthalpy on the crystal lattice constant. Further a material dependent interplay of chemical and strain contributions has been found.

MM 39.3 Thu 16:45 IFW A

Interplay between magnetism and defects in Fe, Cr and their alloys from first principles — •Chu-Chun Fu[1], Romain Soulairol[1], and Cyrille Barreteau[2] — [1]CEA,DEN, Service de Recherche de Metallurgie Physique, 91191 Gif sur Yvette, France — [2]CEA-Saclay, DSM/IRAMIS/SPCSI, 91191 Gif sur Yvette, France

Iron-based alloys, which show complex structural-magnetic phase diagrams, play a major role in metallurgical and nuclear technology. In this work, we investigate, by means of Density Functionnal Theory (DFT), the influence of magnetism on structural and energetical properties of such alloys.

Fist, we give a detailed description of various non-conventional magnetic phases such as spin spiral and spin density waves in bulk Fe and Cr, in particular, we predict the polarization of spin density waves in the ground state of Cr in good agreement with experimental evidence [1].

Then, we report on the properties of defects (vacancies, substitutional impurities and interfaces) in Cr and FeCr alloys with various magnetic configurations. Our results show a significant interplay between magnetism and defects, e.g. stabilization of non-collinear magnetic configurations near both FeCr (110) interface and small Cr clusters in Fe. The dissolution energy of *3d* elements in bcc Fe is also detailed, pointing out the influence of both d-band filling and magnetism, the latter being crucial in the case of Cr in Fe.

[1] R. Soulairol et al., J. Phys. Condens. Matter, 22, 295502 (2010)

MM 39.4 Thu 17:00 IFW A

Superheating Gallium Clusters — •Nicola Gaston[1] and Krista G. Steenbergen[2] — [1]MacDiarmid Institute, IRL, Wellington, New Zealand — [2]Victoria University Wellington, New Zealand

The experimental discovery of superheating in gallium clusters [1] contradicted the clear and well-demonstrated paradigm that the melting temperature of a particle should decrease with its size [2]. However the extremely sensitive dependence of melting temperature on size also goes to the heart of cluster science, and the interplay between the effects of electronic and geometric structure [3]. In the case of gallium, the extreme polymorphism displayed by the bulk metal introduces additional complications. We use our understanding of the dimeric bulk structure of gallium to elucidate the patterns of bonding in the clusters, which also display dimeric structural motifs for small sizes. In particular, the deviation of gallium from the extremely general linear relationship of melting temperature and cohesive energy for elemental solids demonstrates that the low melting temperature of gallium corresponds to the melting of a molecular solid. We present systematic calculations of the melting-like transition in small gallium clusters, and a comparison with aluminium clusters of similar sizes. Finally, we discuss the importance of features of the electronic structure for the melting-like transition.

[1] G. A. Breaux, R. C. Benirschke, T. Sugai, B. S. Kinnear, and M. F. Jarrold, Phys. Rev. Lett. 91, 215508 (2003) [2]P. Pawlow, Z. Phys. Chem. 65, 1 (1909) [3]M. Schmidt, R. Kusche, B. von Issendorff, and H. Haberland, Nature 393, 238 (1998)i

MM 39.5 Thu 17:15 IFW A

Lithium oxide nanoparticles in lithium-air batteries: an ab-initio study — •Nicola Seriani — The Abdus Salam International Centre for Theoretical Physics

Lithium-air batteries may become an attractive solution for energy storage thanks to their high energy density. A key process in this kind of battery is the reversible lithium oxidation at the cathode. To get an atomistic insight into this process, we have performed density functional theory calculations. We show how the resulting oxide phase might be either Li_2O or Li_2O_2, depending on temperature and particle size. At room temperature, Li_2O_2 is the stable phase for particles smaller than 2.5 nm, whereas at larger diameters Li_2O becomes stable. Consequences for battery performance are discussed.

MM 39.6 Thu 17:30 IFW A

Multiscale modeling of nanowire-based Schottky-barrier field-effect transistors for sensor applications — •Daijiro Nozaki[1], Jens Kunstmann[1], Felix Zoergiebel[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062, Dresden, Germany — [2]Division of IT Convergence Engineering and National Center for Nanomaterials Technology, POSTECH, Pohang, Republic of Korea

We developed a theoretical framework for the calculation of charge transport through nanowire-based Schottky-barrier field-effect transistors that is conceptually simple but still captures the relevant physical mechanism of the transport process. Our multiscale model combines two approaches on different lengthscales: (1) the finite element method to calculate the electrostatic potential across the Schottky-contact and (2) the Landauer approach combined with the method of non-equilibrium Green's functions to calculate the electron transmission through the device. Our model correctly reproduces typical I-V characteristics of FETs and we obtained current saturations and high on/off ratios that are in good agreement with the experiment.

MM 39.7 Thu 17:45 IFW A

A molecular dynamics approach to simulate Raman and IR spectra in silicon nanowires — Felix Zörgiebel, •Jens Kunstmann, Daijiro Nozaki, and Gianaurelio Cuniberti — Insitute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

We developed a method to filter phonons from molecular dynamics (MD) simulations based on a density functional tight binding approach. We are able to extract phonon frequencies, polarizations, and q-vectors. Our results for silicon bulk and silicon nanowires show good agreement with experimental data and exceed the accuracy and applicability of the Hesse matrix approach. In particular we are able to determine phonon occupations and temperature effects. Furthermore we filtered Raman, Infrared, and silent modes from MD trajectories via symmetry analysis. This enables us to predict Raman and Infrared spectra of silicon nanowires and explain their origin in terms of phonon polarizations.

MM 39.8 Thu 18:00 IFW A

TDDFT study of the momentum-dependent loss function of palladium — •Stephan Sagmeister[1], Kathrin Glantschnig[1], Gerald Kothleitner[2], Cecile Hebert[3], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben , Austria — [2]Institut für Elektronenmikroskopie und Feinstrukturforschung, TU Graz , Austria — [3]Ecole Polytechnique Federale de Lausanne (EPFL) (Institute of Condensed Matter Physics) , Switzerland

The momentum-dependent loss function of several bulk metals, including palladium, is investigated by means of time-dependent density functional theory (TDDFT) as well as experimental data based on

EELS (electron energy loss spectroscopy) measurements. On the theoretical side, density-functional theory within the full-potential LAPW (linearized augmented planewave) method is employed to obtain the Kohn-Sham band structure, using the exciting code. The framework of TDDFT is utilized within the linear response regime for the calculation of the macroscopic dielectric function and hence the loss function, including crystal local-field effects. The loss function is studied as a function of momentum transfer q for several directions in the Brillouin zone. While TDLDA, or even the independent-particle approximation, can well reproduce the low energy range, for higher energies local-field effects become crucial. For the case of Pd this is reflected in the spectra within the range of 40 to 60 eV, where the local-field effects can reduce the spectral weight by up to 50%. The calculations are in excellent agreement with experimental data.

MM 39.9 Thu 18:15 IFW A

Lead-free piezo-electrics: A combined investigation via synchrotron measurements and first-principles calculations — •Sascha B. Maisel, Henry E. Mgbemere, Rodrigo P. Fernandes, Gerold A. Schneider, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestrasse 15, 21073 Hamburg, Germany

We present structural and chemical investigations of lead-free piezomaterials based on perovskite niobates like $NaNbO_3$, $KNbO_3$, $LiNbO_3$ and their multinary compounds from ab-initio calculations. Since some intrinsic properties of these materials (like ferroelectricity) are very sensitive to cell geometry and the precision of relaxations, the choice of the correct super cells and exchange-correlation functionals is crucial. To make the proper choices, we compare the data from density functional theory with experimental data from both single crystals and sintered ceramics, with very good agreement. The cluster expansion formalism is applied to these DFT results in order to obtain concentration resolved information on short range ordering of the materials. Once the proper short range ordering is known, we are able to calculate piezoelectric response tensors for realistic super cells by means of density functional perturbation theory. The eventual aim of these investigations is to give a quantitative description of the electric and piezoelectric behavior as a function of compound concentration.

MM 39.10 Thu 18:30 IFW A

Superabundant vacancies in fcc metals: A combination of ab-initio, thermodynamic and kinetics approaches — •Roman Nazarov, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

A dramatic increase of the vacancy concentration in a H-rich atmosphere, the so called superabundant vacancy formation, has been experimentally observed in several metals and alloys. In order to study this phenomenon we systematically applied density functional theory to a large set of fcc metals. We found that a large amount of H can be trapped by a monovacancy with, e.g., up to 15 H atoms in an Al vacancy, up to 12 H atoms in the case of Pd and more than 17 H atoms for Pb.

Based on the defect formation energies from DFT calculations, we have constructed a thermodynamic model that determines the equilibrium concentration of point defects as a function of temperature and H chemical potential. By applying this approach we revealed that the vacancy concentration can indeed strongly increase if H is added.

To understand the phenomenon of accelerated self-diffusion in a H-rich atmosphere we coupled the information on the number of vacancies from the thermodynamic treatment with self-diffusion barriers obtained from DFT calculations. Using this approach we found that the self-diffusion coefficient is reduced not only due to the increased vacancy concentration, but also as a result of a H-induced lubricant effect.

MM 39.11 Thu 18:45 IFW A

Mechanism of Hydrogen Binding to Metal-Doped Carbon Nanostructures — •Mina Yoon[1,2] and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Oak Ridge National Laboratory, USA

Using quntum mechanical first-principles calculations based on numerical atom-centered orbitals as all-electron basis functions we study the mechanism of hydrogen binding to metal-doped nanoscale carbons. These materials have been widely studied as potential building blocks for hydrogen storage. We systematically investigate and compare the performance of different approaches in describing the interaction between hydrogen and metals doped on nanocarbons and the importance of the vibrational contribution in the formation enthalpy. The employed approaches include various DFT xc functionals, a semi-empirical approach, and Møller-Plesset perturbation theory. By comparing the chemical potential with that of free hydrogen gas at a finite temperature (T) and pressure (p), we identify the (T,p) conditions for hydrogen absorption/desorption. The vibrational contribution to the chemical potential of hydrogen is prominent for dihydrogen adsorption to metals, where its significance dramatically changes depending on the binding characteristics. This feature is illustrated by the example of metal-doped fullerenes and graphenes.

MM 40: Nanomaterials III

Time: Thursday 16:15–17:30 Location: IFW B

MM 40.1 Thu 16:15 IFW B

Continuous recrystallization and mechanical properties of a C45 steel after high pressure torsion — •Mike Haddad[1,2], JiangLi Ning[2], Ute Hörmann[3], Maxim Murashkin[4], Yulia Ivanisenko[2], and Hans Fecht[1,2] — [1]Institute of Micro and Nanomaterials, University of Ulm, Ulm, Gemany — [2]Institute of Nanotechnology, Karlsruhe Institut of Technology, Karlsruhe, Germany — [3]Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany — [4]IPAM, Ufa State Aviation Technical University, Ufa, Russia

An initial microstructure of C45 steel (Fe, 0.42-0.5% C, 0.5-0.8% Mn, <0.4% Si, <0.045% S, 0.045% P * All in wt%) was modified from ferritic-pearlitic to bainitic through heating at 900°C for 1 hour and quenching in a lead bath at 500°C for 30 min. The steel was processed by High Pressure Torsion (HPT) at room temperature for 3 and 5 rotations, which led to an ultrafine or nano-scale grained structure. Then the material was annealed at 400°C and 450°C for two hours, respectively. TEM observation showed that continuous recrystallization occurred during the annealing. The yield strength and elongation after annealing at 400°C and 450°C were 1277 MPa, 3%, and 1100 MPa, 11%, respectively. Compared with the mechanical properties before annealing, it was revealed that the continuous recrystallization during annealing led to an enhancement of the ductility, but without sacrificing much of the strength.

Funding by the Deutsche Forschungsgemeinschaft and Russian Foundation for basic research is gratefully acknowledged.

MM 40.2 Thu 16:30 IFW B

Martensitic transformation of nanostructured NiTi made by crystallization of a deformation induced amorphous phase — •Martin Peterlechner[1], Christoph Gammer[2], Gerhard Wilde[1], and Thomas Waitz[2] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster — [2]Physik nanostrukturierter Materialien, Fakultät für Physik, Universität Wien, 1090 Wien

Nanocrystalline NiTi shape memory alloys with a tailored grain size are of interest for applications. In this work, bulk nanostructured NiTi was processed by nanocrystallization of an intermediate amorphous phase made by repeated cold rolling (RCR). The structures and their phase stability were studied using transmission electron microscopy and calorimetry. RCR deformation causes grain refinement and amorphization; at high deformation degrees an almost completely amorphous phase is achieved. Upon heating nanocrystallization occurs. Combinations of the deformation degree and annealing condition allow to control the final grain size. Grains are stable up to ~370°C where grain growth occurs. The occurring martensitic phase transformation was analyzed using calorimetry, showing that the grain size strongly impacts the transformation path and temperatures. The transformation from the B2 austenite to the B19' martensite occurs via the intermediate R-phase. The effect of the grain size on the transformation temperature of the R-phase is small; this is in contrast to the transformation to the B19' martensite, which strongly depends on the grain size. With decreasing grain size, both the forward transformation (from B2 to B19') and the reverse transformation shift to lower

temperatures.

MM 40.3 Thu 16:45 IFW B

Melting of faceted Pb nanoparticles — •Anna Moros, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

Melting of confined and nanometer-sized Pb inclusions embedded in a polycrystalline aluminum matrix has been intensively investigated in order to utilize the experimental results obtained on this model system for clarifying the relevance of different models that describe the size dependence of reversible phase transformations. Yet, this phenomenon is still not completely understood. For this reason a study of the melting behaviour of nanometer-sized and faceted Pb particles embedded in an Al matrix based on calorimetry and transmission electron microscopy has been performed. The size distribution of the Pb inclusions was obtained and utilized for the deconvolution of the contributions of different size classes to the total melting signal. Detailed calorimetric analyses revealed that faceted Pb particles melt at elevated temperatures but have reduced melting enthalpy compared to the bulk material. The related thermodynamic consequences are critically discussed.

MM 40.4 Thu 17:00 IFW B

3D imaging of electrostatic potentials in nanostructures with electron holographic tomography — •Wolf Daniel[1], Lubk Axel[2], and Lichte Hannes[1] — [1]Triebenberg Laboratory, Institute of Structure Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]CEMES-CNRS, 29 rue J. Marvig, 31055 Toulouse, France

Electron-holographic tomography (EHT), that is, the combination of off-axis electron holography (EH) with electron tomography (ET), allows the quantitative 3D mapping of electrostatic potentials and magnetostatic vector fields with a resolution of a few (5-10) nanometers. The 3D potential offers the outer (morphology) and inner structure, as well as the mean inner potential (MIP) of the nano object. This is shown on epitaxially grown nanowires (NWs) of GaAs and AlGaAs. The 3D morphology is studied using the corresponding iso-surfaces of the 3D potential: The facets on the nanowires surface allow conclusions about the crystalline structure. Moreover, the reconstructed 3D potential of a AlGaAs/GaAs NW clearly shows its core/shell structure due to the MIP difference between GaAs and AlGaAs of $0.61\,V$. For doped semiconductor structures with pn-junctions (e.g. transistors) the potential distribution, reconstructed by EHT, also provides access to the built-in voltage across the pn-junction. The built-in voltage ΔV_{pn} can be analyzed in 3D and measured without projection and surface effects (e.g. dead layers) within the sample. The measurements of ΔV_{pn} in three needle-shaped specimens, prepared by FIB, yield for two silicon needles $1.0\,V$ and $0.5\,V$, and for a germanium needle $0.4\,V$.

MM 40.5 Thu 17:15 IFW B

Elastic properties and deformation of mesoporous glass during sorption of argon — •Klaus Schappert and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus E2.6, 66123 Saarbrücken, Germany

Sorption of atoms or molecules in porous matrices can induce stress and thus a noteworthy deformation of the material. Here, we present measurements of the length change of mesoporous Vycor glass during isothermal adsorption and desorption of argon both above and below its freezing point. We compare the behaviour of this macroscopic length change with the elastic properties of the adsorbed argon, that we evaluate via ultrasonic measurements. Thereby, we are able to relate the deformation of the porous sample to the microstructure of the adsorbate.

MM 41: Topical Session Diffussionless Transformations II

Time: Thursday 16:15–17:45 Location: IFW D

MM 41.1 Thu 16:15 IFW D

Martensitic transformations in thin epitaxial films of the NiTi shape memory alloy — •Joerg Buschbeck, Jason Kawasaki, Alexander Khozanov, and Chris Palmstrom — ECE Department, University of California, Santa Barbara, US

Phase formation and martensitic transformations are studied on molecular beam epitaxy (MBE) grown Ni-Ti films over a wide range of Ti contents from 43 to 56 at.%. Ordering of the B2 phase is investigated as function of growth temperature. Lattice mismatch stabilizes the NiTi B2 phase in a tetragonally distorted structure. Despite the epitaxial interface constraining the only 35 nm thick films, we observe reversible martensitic transformations in temperature dependent X-ray diffraction and resistivity. Ti-content and epitaxial interface control the transformation temperatures. In similarity to the B2-R-B19' sequence in bulk, a two-stage martensitic transformation is observed. This transformation occurs without tilt of the normal lattice vector, as temperature dependent reciprocal space mappings show.

MM 41.2 Thu 16:30 IFW D

Smart Heusler materials from first-principles calculations — •Peter Entel, Antje Dannenberg, Mario Siewert, and Markus E. Gruner — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

The interplay of structural and magnetic phase transitions vastly determines the properties of ternary intermetallics such as X_2YZ Heusler alloys. Here, X and Y are ransition metal elements and Z is an element from the III-V group. In order to give a precise prescription of the possibilities to optimize the magnetic shape memory and magnetocaloric effects of these alloys, we use density functional theory calculations. From these calculations we can infer the martensitic driving forces and reveal the dominant role of the *d*-electrons in the formation of both, the different martensitic structures as well as the different magnetic spin orderings as a function of the atomic composition. In particular, we outline how one may find new intermetallics which show higher Curie and martensitic transformation temperatures when compared with the prototypical magnetic-shape memory compound Ni_2MnGa. Higher operation temperatures are needed for technological applications. On the other hand, the optimization of the magnetocaloric effect is strongly related to find alloys for which the magnetic and structural phase transitions merge in a narrow temperature interval. This allows for larger adiabatic temperature changes across the transitions in an external magnetic field.

MM 41.3 Thu 16:45 IFW D

Ab initio derivation of chemical trends in the phase temperatures of Ni_2MnGa-based shape memory alloys — •Ali Al-Zubi, Tilmann Hickel, and Jörg Neugebauer — Max Planck Institut für Eisenforschung, 40237 Düsseldorf

Since martensitic phase transitions are essential for the shape memory effect, their dependence on the chemical composition is of utmost importance for the application of these alloys. In this study we systematically investigated chemical modifications of the magnetic Heusler alloy Ni_2MnGa, with a particular focus on an excess Ni content. We combine density functional theory with thermodynamic concepts in order to derive accurate temperature dependencies of the free energies for the austenitic, pre-martensitic and martensitic phase. Vibrational excitations are treated in the quasiharmonic approximation and magnetic excitations are considered in a fixed-spin moment approach, yielding a delicate interplay of these two degrees of freedom. Particular care has been taken to determine the shuffling structures related to soft phonons. Using this approach we were able to successfully describe the phase transitions for different chemical compositions. In very good agreement with experiment, we find an increase of the martensitic phase transition temperature with x in $Ni_{2+x}Mn_{1-x}Ga$ and revealed a sensitive dependence of this behaviour on the Curie temperature of the system. Further, a strong dependence of the pre-martensitic phase stability on the Ni content was resolved. The information have been combined in temperature-dependent phase diagrams.

MM 41.4 Thu 17:00 IFW D

First-principles investigation of the magnetic shape memory system Co-Ni-Ga — •Mario Siewert, Markus E. Gruner, Antje Dannenberg, and Peter Entel — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

The magnetic shape memory (MSM) system Ni-Mn-Ga still has limited applications because the operating temperatures are not suitable for many practical devices. Hence, the search for new ferromagnetic shape memory compounds is not only of scientific but also of industrial importance. One approach to find new MSM alloys are Heusler compounds based on Co. Here, we present first-principles results for the Co-Ni-Ga system. In particular, the structural, electronic and dynamic properties of stoichiometric Co_2NiGa and off-stoichiometric compositions have been investigated using density functional theory. Our results reveal that there is a competition between tetragonal distorted and bcc-like structures. In addition, a competition between different structural orderings, namely the regular Heusler structure and the so called inverse Heusler structure, occurs. In advance, no phonon softening along the [110] direction is found for Co-Ni-Ga in agreement with neutron scattering measurements. This is supported by the electronic structure which reveals no sign of Fermi surface nesting.

MM 41.5 Thu 17:15 IFW D

Competing structural ordering tendencies in new high-TC ferromagnetic Fe-Co-based Heusler alloys from ab initio investigations — •Antje Dannenberg[1], Markus Gruner[1], Manfred Wuttig[2], and Peter Entel[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Materials Science and Engineering,University of Maryland, College Park, MD 20742, USA

Fe-Co-based Heuslers are candidates for new ferromagnetic shape memory alloys (FSMA) as they promise higher operation temperatures compared with prototype Ni2MnGa. Of interest are also the corresponding binary systems FeZn and Fe3Ga which show a huge magnetostriction. We present results of ab initio and Monte Carlo calculations regarding structural, magnetic, and electronic properties of Fe2CoGa1-xZnx alloys in conventional X2YZ and inverse (XY)XZ Heusler structures. All systems exhibit high Curie temperatures TC. The preference of the cubic inverse structures is believed to originate from the bcc-like environment of two inequivalent Fe atoms and their strong hybridization with the Co- states. Weakening the Co-Fe hybridization by substitution of Ga by Zn reduces this preference and leads to higher TC but simultaneously reduces the miscibility. Despite the strong spin-dependent Fe-Co hybridization we find a localized character of the spin moments. Extraordinary Z-elements like Cu, Ag, and Au or further enhancement of the Zn content induces a martensitic instability also in the inverse structures. Thus, we conclude that it is possible to find new FSMA with rather high Curie temperatures.

MM 41.6 Thu 17:30 IFW D

Twin boundary rearrangement in magnetic shape memory alloys studied with a phase-field model — •Frank Wendler, Christian Mennerich, Marcus Jainta, and Britta Nestler — IMP, Karlsruhe University of Applied Sciences

The observed large magnetic field induced strain (MFIS) in magnetic shape memory alloys is characterized by a structural rearrangement of martensite variant fractions. The complicated interdependency of microstructure - stress - magnetic field in the alloy Ni2MnGa motivates this numerical study. The displacive phase transition in the free boundary problem is treated by a phase-field model, based on the formulation of chemical, micromagnetic and magneto-elastic free energy densities. For the isothermal situation of martensite nucleation in the parent phase and twin boundary motion in the martensitic state, order parameters for variants and parent phase are introduced and related to their eigenstrain. The parameters are evolved according to Allen-Cahn dynamics, whereas a time dependant wave equation is solved for the field of elastic displacements. The magnetization field is updated by solving the Landau-Lifshitz-Gilbert equation with a geometric integration scheme. First, a verification of the variational approach is given for the subproblems of either magnetic or elastic fields interacting with the variant structure. Then, we focus on the reversible transformation process in single crystals, where the coupled evolution of magnetic domains and twin variants is studied and examples for resulting magnetization and strain reaction are given. An extension of the approach to treat polycrystalline materials is discussed.

MM 42: Functional Materials I

Time: Thursday 17:45–19:00 Location: IFW B

MM 42.1 Thu 17:45 IFW B

Correlation of structural properties and electrochemical characteristics of carbon aerogel electrodes — •Volker Lorrmann[1], Gudrun Reichenauer[1], Vladimir Dyakonov[1,2], and Jens Pflaum[1,2] — [1]Bavarian Center of Applied Energy Research e.V. (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius-Maximillians-University of Würzburg, 97074 Würzburg

In electrochemical double-layer capacitors (EDLC) the energy is stored in the electrochemical double-layer interface between the electrode surface and the electrolyte solution. The capacitance of EDLCs and rate capability depend on the porous nanostructure of the electrodes. Carbon aerogels, based on sol-gel derived organic precursors, are promising candidates for EDLC electrodes because of their tunable nanostructure (e.g. pore- and particle size). For the same reason these materials also represent excellent model systems for the investigation of correlations between structural properties and electrochemical characteristics. We prepared carbon aerogel EDLC electrodes with different primary particle sizes using different catalyst concentration in the starting solution. Scanning electron microscopy measurements of the carbons show, that the particle size and hence the interparticular pores are varied between several ten nm up to some μm. Electrochemical investigation was performed by cyclic voltammetry and impedance spectroscopy in different electrolyte solutions. The relationship between the nanostructure and the electrochemical performance of the carbon aerogel is discussed.

MM 42.2 Thu 18:00 IFW B

Structure of layered covalent organic frameworks — •Binit Lukose, Agnieszka Kuc, and Thomas Heine — School of Engineering and Science, Jacobs University Bremen, Bremen, Germany

Covalent-Organic Frameworks (COFs)[1] are a new family of 2D and 3D highly porous and crystalline materials built of light elements, such as boron, oxygen and carbon. For all 2D COFs, AA stacking arrangement has been reported on the basis of experimental powder XRD patterns, with the exception of COF-1 (AB stacking). The AA stacking arrangement maximizes the attractive London dispersion interaction between the layers, which is the dominating term of the stacking energy. At the same time, AA stacking always results in a repulsive Coulomb force between the layers due to the polarized connectors. In this work[2,3], we show that a set of reported and hypothetical 2D COFs are considerably more stable if their stacking arrangement is either serrated or inclined, and layers are shifted with respect to each other by ~1.4 Å. These structures are in agreement with to date experimental data, including the XRD patterns, and lead to a larger surface area and stronger polarization of the pore surface.

[1] Porous, crystalline, covalent organic frameworks. A. P. Cote, O. M. Yaghi, et al Science 310 (2005) 1166-1170

[2] Structure of layered covalent organic frameworks. B. Lukose, A. Kuc, T. Heine, Chem. Eur. J. (2010) accepted for publication.

[3] On the reticular construction concept of covalent organic frameworks. B. Lukose, A. Kuc, J. Frenzel, T. Heine, Beilstein J. Nanotechnol. 1 (2010) 60-70.

MM 42.3 Thu 18:15 IFW B

Study of the degradation of conjugated polymers using scanning probe microscopy — •Esha Sengupta, Anna L. Domanski, Stefan A.L. Weber, Maria B. Retschke, Hans Jürgen Butt, and Rüdiger Berger — Max Planck Institute for Polymer Research, Mainz, Germany

A major problem for applications of conjugated polymers in organic photovoltaics is their limited life-time [1]. Degradation occurs when these are exposed to sunlight, oxygen and water. Recent studies have reported changes in the open circuit voltage (Voc) and short circuit current (Jsc) in fabricated organic solar cells as estimates of degradation [2]. However, in these studies, device fabrication and optimization of the processing steps are time consuming. Since the morphology of organic solar cells needs to be controlled on a nanometer scale due to small exciton pathways, Scanning Probe Microscopy (SPM) provides a valuable tool to study topographic and electronic effects. Here, we present an SPM based method to study degradation of con-

jugated polymers without the need to fabricate devices. Changes in the surface potential and conductivity due to degradation of the active layer of solar cells were investigated using Kelvin Potential Microscopy (KPM) and conductive Scanning Force Microscopy (c-SFM). These changes have been related to the Voc and Jsc changes upon degradation. We expose the active layer directly to simulated sunlight and varying amounts of oxygen and humidity while partially covering it with a grid. [1] Krebs, F.C. et al., Chemistry of Materials, 2005, 17, 5235 [2] Seemann, A., et al., Organic Electronics, 2009, 10, 1424.

MM 42.4 Thu 18:30 IFW B

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

In-situ XRD measurements of hydrogen absorption behavior were done for nano-crystalline Mg thin films at room temperature. 20 nm Pd-capped nanocrystalline Mg films of different thicknesses were prepared in an UHV chamber, by means of ion beam sputter deposition under Ar-atmosphere at the pressure of 2,2*10E-4 mbar. The Mg films were deposited on Si (100) substrates. XRD measurements using a Phillips X-Pert diffractometer with Co-K alpha radiation were performed before and after hydrogenation in order to check the phase transition and the change of the sample texture. In-situ XRD measurements have been done at the HASYLAB synchrotron facility in Hamburg and at European Synchrotron Facility in Grenoble. Changes of the resistivity during hydrogenation were also monitored by four-point measurement, during electrochemical- and gas pressure hydrogen loading. The diffusion coefficient of hydrogen in nano-crystalline Mg thin films at room temperature is estimated from in-situ synchrotron XRD measurements and compared with the results of electrochemical hydrogen permeation measurements. The impact of grain boundaries on the hydrogenation properties is discussed. Financial support by the DAAD, HASYLAB and the ESRF is gratefully acknowledged.

MM 42.5 Thu 18:45 IFW B

Investigation of Lithium diffusion in sputtered layers of lithium titanat — •Fabian Wunde and Guido Schmitz — Institut für Materialphysik, WWU Münster, Deutschland

Lithium titanate (LTO) is used as an anode material for lithium ion batteries, as it reveals both, electronic as well as Li-ion conductivity. To investigate its ionic properties, ion-beam sputter-deposited thin films of LTO have been analysed by means of galvanostatic charge-discharge measurements. It has been observed that the measured charge capacities show a strong dependence on the charge/discharge current densities, i.e the charge capacity decreases when increasing the current. In order to explain this decrease in capacity, the kinetics of Li insertion into the LTO films is described by diffusion. Solving Fick's diffusion law with finite diffusion space while assuming a constant electrical current as boundary condition, leads to theoretical concentration profiles. Subsequent combination of these profiles with the well-known Nernst equation shows that the observed loss of capacity is due to a gradient of the Li concentration and therefore depends on the diffusion coefficient of Li in LTO. By evaluating the measured capacity loss as a function of current the diffusion coefficient is determined.

MM 43: Mechanical Properties II

Time: Thursday 18:00–19:00 Location: IFW D

MM 43.1 Thu 18:00 IFW D

In-situ micro-cantilever tests to study the fracture properties of NiAl — •Farasat Iqbal, Johannes Ast, Karsten Durst, and Mathias Göken — Institute of General Materials Properties, Department of Materials Science & Engineering, University of Erlangen-Nürnberg, Germany

In recent years the nanomechanical testing of materials becomes an important tool to test the materials at micron or even sub-micron scale with the help of different methods. In order to understand mechanical behavior of the bulk materials at micron or sub-micron scale different existing methods including nanoindentation , micro-tensile, bulge test , micro-compression and micro-cantilever fracture test are used on different material systems. In order to understand the relation between micron scale fracture toughness to that of the bulk materials, we carried out in-situ micro-cantilever tests on anisotropic NiAl-single crystals. The reason for choosing NiAl is its brittle nature and the macroscopic fracture toughness using ASTM E399 standard has been already investigated and reported in literature. NiAl possess two orientation namely hard <101> & soft <100> and the macroscopic fracture toughness measured using ASTM 399 standard ranges 3-4 MPa m1/2 for soft orientations and 5-7 MPa m1/2 for hard orientations. Hence the micro cantilever method was used to investigate the orientation dependent fracture toughness of NiAl at micron scale and its possible relation to the macroscopic fracture toughness is also discussed.

MM 43.2 Thu 18:15 IFW D

The fracture toughness of silicon nitride thin films of different thicknesses as measured by bulge tests — •Benoit Merle and Mathias Göken — Department of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, Germany

A bulge test setup was used to determine the fracture toughness of amorphous low pressure chemical vapor deposited (LPCVD) silicon nitride films with various thicknesses in the range of 40 to 108 nm. The method used for this measurement relied on a special sample preparation with a Focused Ion Beam (FIB), in which a crack-like slit of a defined length was introduced in the center of a rectangular freestanding membrane. The membrane was then deformed in the bulge test until failure occurred, and the fracture toughness KIC of the film was calculated from the pre-crack length and the stress at failure. It was shown that the membranes were in a transition state between pure plane-stress and plane-strain, which however had a negligible influence on the measurement of the fracture toughness, because of the high brittleness of silicon nitride and its low Young's modulus over yield strength ratio. The fracture toughness KIC was measured to be constant at 6.3 +/- 0.4 MPa m1/2 over the whole studied thickness range, which compares well with bulk values. This means that the fracture toughness, just as the Young's modulus, is a size independent quantity for LPCVD silicon nitride. This presumably holds true for all amorphous brittle ceramic materials.

MM 43.3 Thu 18:30 IFW D

Mechanical Behaviour of Layered Nanocomposites — •Inga Knorr[1], Susanne Seyffarth[1], Tobias Liese[1], Nicolas Cordero[2], Hans-Ulrich Krebs[1], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Centre des Matériaux, Mines Paris, Paristech

Multilayer thin films with dimensions at the nanometer scale represent a technologically important class of materials which can offer improved mechanical properties as a result of composite, interface and size effects. Here, sample series composed of polycrystalline metal and amorphous layers are investigated, with the goal of understanding the size-dependence of the layer mechanical properties as well as the deformation and failure modes of nanoscale composites. The specific samples have layer thicknesses between 5 and 300 nm and consist of Cu/Polycarbonate, Ti/amorphous ZrO_2, and Cu/amorphous $Pd_{78}Si_{22}$ layers. Mechanical characterization is performed using Berkovich nanoindentation as well as micro-compression tests. Sample morphologies in the undeformed and deformed states are investigated with SEM and TEM. The three sample sets show some common trends in the mechanical behavior. For example, the metal layers show a slight increase in strength with decreasing thickness and grain size, but the effect is much weaker than expected. In addition, the samples often fail by localized shear band formation, which may be attributed to plastic strain induced weakening at the layer interfaces. Explanations for these trends as well as possible tactics for improving the mechanical performance of multilayer films will be discussed.

MM 43.4 Thu 18:45 IFW D

Micro- and Nanostructure Characterization Imaging of TWIP Steels — •Leonardo Batista, Ute Rabe, and Sigrun Hirsekorn — Fraunhofer IZFP, Campus E3 1, 66123 Saarbrücken, Germany

New design concepts for the construction of advanced light-weight

and crash resistant transportation systems require the development of high strength and supra-ductile steels combined with enhanced energy absorption and reduced specific weight. TWIP (Twinning Induced Plasticity) steels have excellent mechanical properties combining high strength levels (Rm > 1000 MPa) with a large uniform elongation (Au > 50%). These properties are a direct consequence of intensive mechanical twinning resulting in a high sustained degree of strain-hardening. The mechanisms and the interaction of the mechanical twinning with the microstructure which leads to such outstanding mechanical properties are, however, not well understood. In order to characterize the microstructure and probe the local material properties combined studies using EBSD (Electron Backscattering Diffraction) and AFAM (Atomic Force Acoustic Microscopy) as well as TEM (Transmission Electron Microscopy) have been used.

MM 44: Functional Materials II

Time: Friday 10:30–13:15 Location: IFW A

MM 44.1 Fri 10:30 IFW A

'The wake of Hydrogen in V, Nb and Ta at elevated temperatures: Irrreversibility and non-central forces revisited. — •Franz Reidinger — 3 Hadley Way Morristown NJ 07960 USA

At elevated temperatures U and Do of the Arrhenius equation for diffusion describe the amplitude and relaxation rate, respectively, of the stern wave wake of H. The key evidence for this hypothesis is the close correlation between the isotope dependence of U derived from measurements of the Gorsky effect 1) and the shear distortion of the orthorhombic phases of NbH(D) and TaH(D). The isotope dependence of U can be described in closed form: U=axsqrt(M)+bxsqrt(m), where M and m are the atomic weights of host metal and H isotope: a and b are 7.4 and 37 for Nb and Ta, and 0 and 55 for V, respectively, in units of meV. I explain this correlation in two steps: a) the cubic symmetry of the nearest neighbor strain field 2) of the interstitial H is the result of a dynamic superposition, possibly caused by a JT resonance 3), of two orthorhombic variants of ordered NbH0.75 and b) the successful characterization of the diffusion process as jump diffusion 4) eliminates the transition state from considerations. 1)Z Qi, J Voelkl, R Laesser and H Wenzl: J.Phys.F 13, 2053 (1983) 2)G Bauer, E Seitz, W Schmatz and H Horner: Sol. State Comm. 17, 161 (1975) 3)GC Abell: J.Phys.F 12, 1143 (1982) 4)V Lottner, A Heim and T Springer: Z.Physik B 32, 157 (1979)

MM 44.2 Fri 10:45 IFW A

Atom probe tomography analysis of deuterium distribution in V-Fe alloy film — •Ryota Gemma[1], Talaat Al-Kassab[2], Reiner Kirchheim[1], and Astrid Pundt[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077, Göttingen, Germany — [2]Division of Physical Sci.& Eng., King Abdullah University of Science & Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

In hydrogen-metal systems, investigation of hydriding properties in reduced dimension has been one of the important issues for materials development in the field of hydrogen storage and sensor applications. Atom Probe Tomography (APT) has opened up a new quantitative approach to demonstrate deuterium (D) distribution in metals. In our previous studies, it has been shown that analysis temperature in the APT analysis and oxygen-exposure of D-loaded specimen exert a major influence on D distribution. These impacts are related to diffusion behavior of D. A reliable analysis of D distribution can be achieved only in the case that the D-diffusion is suppressed. In this study, lateral and depth distribution of D in V-Fe alloy film was investigated by APT at 20 - 30 K. In the analysis of V-Fe5at% film of 10 nm-thickness deposited on a W substrate performed at 30 K, the film loaded with 0.2 Pa deuterium gas showed an average D concentration of 0.23(8) D/Metal, which was in good agreement with the expected concentration of 0.31 D/Metal. An enrichment of D near the V/W interface was observed regardless of analysis temperature, which is explained by the presence of D-trapping effect at misfit dislocations.

MM 44.3 Fri 11:00 IFW A

Blister formation on polycrystalline tungsten due to low-energy deuterium plasma loading — •Armin Manhard, Klaus Schmid, Wolfgang Jacob, Martin Balden, and Stefan Lindig — Max-Planck-Institut für Plasmaphysik, EURATOM Assoziation, Boltzmannstr. 2, 85748 Garching

When polycrystalline tungsten is loaded with deuterium due to plasma implantation with ion energies well below the sputtering threshold but with a high ion flux, the surface morphology of a well-polished specimen can change dramatically. This can be attributed to the supersaturation of the material with deuterium during plasma implantation. Depending on tungsten microstructure, ion flux and specimen temperature, various surface structures such as blisters and other protrusions appear. Their size ranges from microns to tens of microns and each one features a subsurface cavity. These cavities are typically located orders of magnitude deeper than the stopping range of the implanted ions.

This presentation focuses on the formation of blisters on rolled and subsequently polished and stress-relieved tungsten. The abundance and size distribution of the blisters is discussed depending on the specimen temperature. The influence of the initial surface morphology such as, e.g., surface roughness is also addressed. The influence of the tungsten microstructure is examined by investigating recrystallized and subsequently implanted tungsten specimens. In this context, the formation of different types of protrusions which appear on the surface of recrystallized tungsten for very high ion fluxes is also discussed.

MM 44.4 Fri 11:15 IFW A

Combined impact of microstructure and mechanical stress on PdHc thin films electrical resistivity — •Stefan Wagner and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Physical properties of metal thin films strongly depend on their microstructure and stress state. [1] Palladium hydrogen (PdHc) thin films are used as a model system to determine the impact of microstructure and mechanical stress release on the electrical resistivity of thin film metals and alloys that undergo structural phase transitions. The results are compared with bulk resistivity models. Nanocrystalline, multi-oriented and epitaxial films in the thickness range from 5 nm to 2 μm are investigated, yielding initial terminal resistivities of 152 - 200 Ωnm. The hydrogen-related resistivity changes of epitaxial films are shown to approach the predicted α-phase bulk increment $\Delta\rho/\Delta$cH = 451 Ωnm, while hydrogen trapping in nanocrystalline films strongly reduces the resistivity response. In the two phase field the resistivity is shown to be modified by the sterical distribution and geometry of the hydride precipitates, yielding different proportions of serial and parallel conduction. Film delamination from the substrate strongly reduces the resistivity increment due to the Gorsky effect. [2,3]

[1] Wagner S, Pundt A: APL 2008;92:051914. [2] Wagner S, Pundt A: Acta Mat 2010;58:1387. [3] Wagner S, Pundt A: Acta Mat, accepted.

MM 44.5 Fri 11:30 IFW A

Positron lifetime measurements for monitoring vacancies and vacancy clusters in hydride forming free standing Mg films. — •Luca Ravelli[1], Werner Egger[1], Günther Dollinger[1], Roberto Brusa[2], and Riccardo Checchetto[2] — [1]Institut für Angewandte Physik und Messtechnik, Universität der Bundeswehr München, Neubiberg, Deutschland — [2]Dipartimento di Fisica, Università degli Studi di Trento, Trento, Italy

Pd-capped free-standing Mg-based film samples (thickness 10 micrometers) were produced by r.f. magnetron sputtering[1]. The presence of vacancies and the formation of vacancy clusters were studied in the as-prepared sample and in samples submitted to 1, 2, 4 and 8 H2 absorption and desorption cycles by positron annihilation lifetime spectroscopy. For this task a monoenergetic pulsed positron beam of variable energy is necessary to control the implantation depth of the positrons and to depth-profile the defect structure in the Mg films. The measurements were performed with the Pulsed Low Energy Positron System (PLEPS)[2] at the high intensity positron source NEPOMUC (NEutron-induced POsitron source MUniCh) of the research reactor FRM II. Disappearence of vacancies due to their clustering was observed after the second H2 sorption cycle.

[1] N. Bazzanella et al., Appl. Phys. Lett. 85 (2004) 5212-5214.
[2] P. Sperr et al., Appl. Surf. Science 255 (2008) 35-38.

MM 44.6 Fri 11:45 IFW A

Nuclear Magnetic Resonance study of $LiMnPO_4$ with different Li concentrations — •Christian Schmidt, Hans-Joachim Grafe, Nadja Wizent, Lothar Dunsch, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

$LiMnPO_4$ is a promising material for building the cathode of Li-ion batteries due to its high stability and large cation mobility. Yet, the mobility of the Li-ions in this material is not well understood. Here, we present ^{7}Li and ^{31}P Nuclear Magnetic Resonance (NMR) measurements on Li_xMnPO_4 single crystals for different doping levels (x=0.6, x=0.8, and x=1). NMR is a powerful tool to investigate the microscopic ionic jump processes rather than the macroscopic material transport. The nuclear spin lattice relaxation rate, $1/T_1$, and the linewidth, σ, of the resonance lines show characteristic temperature dependencies related to the ionic jump processes that set in at a certain energy or temperature, respectively. The advantage of the use of single crystals is that the linewidth is not broadened by a distribution of linewidths as in a powder sample, but can show a fine structure that could be related to different sites in the crystal. Furthermore, single crystals allow for an orientation dependent investigation of the Li-ion mobility, where certain crystal orientations are preferred by the Li-cations.

MM 44.7 Fri 12:00 IFW A

$SrTi_{1-x}Nb_xO_{3-\delta}$ glass-ceramics as oxidic thermoelectric materials — •Julian Lingner[1,2], Martin Letz[1], and Gerhard Jakob[2] — [1]Schott AG, Hattenbergstraße 10 Mainz — [2]Johannes Gutenberg-Universität Mainz

Thermoelectrics are materials that convert waste heat into electrical power. The quality of a thermoelectric substance is characterized by the dimensionless figure of merit $ZT = \frac{S^2\sigma}{\kappa}T$. One essential advantage of glass-ceramics is their low thermal conductivity κ together with the high temperature stability of up to 700°C. The crystal phase $SrTiO_3$ is a wide bandgap semiconductor, doping with niobium and with oxygen vacancies shifts the Fermi level into the donor band resulting in a insulator-metal transition. Furthermore, nanoscale structure offers a possibility to improve the performance and allows to adjust the material to the required application. Nano crystalline conducting crystal grains effectively reduce the dimensionality of the conducting material, which allows to modify the density of states and therefore the Seebeck coefficient S and the electrical conductivity σ, thus increasing the thermoelectric figure of merit. Using a short range infrared heat treatment, a controlled crystallization in the glass samples can be induced so that nanoscale $SrTiO_3$ crystals are formed in the glass-ceramic. We show results of thermoelectric properties of first glass-ceramic systems containing doped $SrTiO_3$.

MM 44.8 Fri 12:15 IFW A

Hybrid electrode for electrochemical capacitors consisting of a MnO_2 infiltrated carbon aerogel — •C. Weber[1], V. Lorrmann[1], G. Reichenauer[1], V. Dyakonov[1,2], and J. Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical capacitors (EC) bridge the gap between conventional capacitors with high power but low energy density and batteries with high specific energy density but rather low power density. There are two types of EC: Double-layer capacitors, based on the electrostatical storage of charges in the Helmholtz-layer between the electrolyte and the electrode of large surface area, the latter typically consisting of activated carbon. In pseudocapacitance capacitors charging is of faradaic nature, e.g. by redox processes in oxides of transition metals. We have prepared EC hybrid electrodes by infiltrating a carbon aerogel with manganese oxide (MnO_2).

Variations in structure of the carbon aerogel backbone and the amount of deposited MnO_2 were characterized electrochemically and structurally. Due to the MnO_2 deposition, the gravimetric capacitance was augmented by a factor 2, whereas the volumetric capacitance was increased by a factor 5, compared to the capacitance of the bare carbon aerogel, respectively. Remarkably, these findings are independent of the concentration of MnO_2 in the precursor.

Financial support by Deutsche Bundesstiftung Umwelt is gratefully acknowledged.

MM 44.9 Fri 12:30 IFW A

Stability of polymer-ceramics interfaces in hybrid materials: The role of coupling agents and surfactants — •Wolfgang Heckel, Kristina Brandt, Tobias C. Kerscher, Sascha B. Maisel, Gerold A. Schneider, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

The mechanical properties of hierarchically structured materials like ceramics-polymer systems heavily depend on the composition of the interface materials and the choice of an optional adhesive. As an example we have investigated the Titaniumdioxide-PMMA system by application of different experimental techniques. In order to control the properties of the system, we use density functional theory to analyze the stability of this interface and compare different surfactants, adhesives and coupling agents. Indeed, a detailed knowledge of the local electronic and energetic behaviour at the polymer-agent-ceramics interface is crucial. The resulting energetics and electronic properties depend on both the agent-ceramics and the agent-polymer bond stength.

MM 44.10 Fri 12:45 IFW A

Magnetoelectric FeCoBSi/PVDF bilayers — •Kerstin Meurisch, Robert Jahns, Eric Woltermann, Thomas Strunskus, Vladimir Zaporojtchenko, and Franz Faupel — Tecnical Faculty of the University of Kiel, Germany

In Magnetoelectric composites magnetostrictive and piezoelectric materials are combined in a way that changes in the dimension of the magnetostrictive material by an external magnetic field will lead to a measurable polarization change of the piezomaterial. It was already demonstrated that laminates fabricated by gluing of a FeCoBSi foil to a PVDF (polyvinylidene fluoride) foil provide a fairly high magnetoelectric response [1], but downsizing and integration into devices is rather complicated. To avoid these problems and to achieve a better mechanical coupling at the metal-polymer interface we deposited the FeCoBSi directly onto a piezoelectric PVDF foil by DC magnetron sputtering. An in situ applied magnetic bias field was used to improve the magnetic field direction sensitivity. The influence of the substrate preparation, sensor design and sputter parameters on the magnetoelectric output signal will be discussed.[1] Zhai, J.; Dong, S.; Xing, Z.; Li, J. & Viehland, D;. Giant magnetoelectric effect in Metglas/polyvinylidene-fluoride laminates; Appl. Phys. Lett.; 2006, 89, 083507

MM 44.11 Fri 13:00 IFW A

Novel method to produce catalysts for oxygen reduction re- action by dual plasma process — •Christian Walter[1], Volker Bruser[1], Antje Quade[1], Klaus-Dieter Weltmann[1], Kurt Kummer[2], and Denis Vyalikh[2] — [1]INP Greifswald e.V. Felix-Hausdorff-Str. 2 17489 Greifswald — [2]TU Dresden Inst. für Festkörperphysik Helmholtzstraße 10 01069 Dresden

Polymer electrolyte membrane fuel cells (PEMFCs) have been recognised as a potential future power source for zero emission vehicles [1]. Today, Pt is the only efficient catalyst for the oxygen reduction reaction (ORR) in PEMFCs. But for reasons of availability and cost efficiency there is a great desire to replace Pt with inexpensive and abundant catalysts (Non-noble-metal catalysts (NNMCs)). Metal (Co/Fe)/N/C composites have emerged as the most promising alternatives within the NNMcs. Those composites are either prepared by pyrolisation of Co- or Fe-N_4-macrocycles at high temperatures in an inert atmosphere or by introducing the metal and the nitrogen precursors separately onto carbon support and subsequent pyrolisation [2]. But it has also been shown that metal-polymer-composites can be produced by a dual PECVD/PVD process [3]. In this contribution, such a dual process is used with pyrrole as the polymer and cobalt as metal to obtain catalytically active composites. Advantages and shortfalls of this technology are discussed.

[1] R. Bashyam and P. Zelenay; *Nature*, **2006**, 443,63-66
[2] F. Jaouen et al.; *ACS Appl. Mater. Interfaces*, **2009**, 1 (8), 1623
[3] C.Walter et al.; *Plasma Process. Polym.*; **2009**, 6, 803-812

MM 45: Topical Session Heterogeneous Nucleation II

Time: Friday 10:30–11:45 Location: IFW B

MM 45.1 Fri 10:30 IFW B

Grain refinement of TiAl-based alloys: experiments and model calculation — •Daniel Gosslar[1], Robert Günther[1], Christian Hartig[1], Florian Pyczak[2], Andreas Stark[2], Ulrike Hecht[3], and Rüdiger Bormann[1] — [1]Hamburg University of Technology, Institute of Material Science and Technology, 21073 Hamburg, Germany — [2]Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research, 21502 Geesthacht, Germany — [3]ACCESS e.V., 52072 Aachen, Germany

Turbine blades of TiAl-based alloys are on the verge of series production. The major advantages of these alloys are their good mechanical properties up to at least 800 °C and the relatively low density. Thereby it becomes possible to replace heavier Ni-based alloys in order to save weight and reduce fuel consumption of aircraft engines. Microstructure refinement of TiAl-based alloys is an important issue of concern. It can be achieved by several distinct ways, depending on alloy composition. One possible way offers particle inoculation of the melt using adequate boron / boride additions. Conventional casting experiments are used to study the effect of boride inoculation on the as cast microstructure. The boride phases are investigated by transmission electron microscopy and synchrotron diffraction experiments. For the first time a metastable monoboride is identified in a high boron containing (> 2 at.% B) Ti-45Al (at.%) alloy. The nucleation potency of this boride is evaluated by the crystallographic model of P.M. Kelly and M.-X. Zhang. The grain size evolution is analyzed using the free growth model of L.A. Greer for heterogeneous nucleation.

MM 45.2 Fri 10:45 IFW B

Peritectic solidification in Al-Ni alloys — •Hai-Lin Chen and Rainer Schmid-Fetzer — Institute of Metallurgy, TU Clausthal, Robert-Koch-Str. 42, D-38678 Clausthal-Zellerfeld, Germany

This work aims at a better understanding of the mechanism of peritectic solidification, including the four stages of heterogeneous nucleation, peritectic reaction, peritectic transformation and direct growth of the peritectic phase, and their roles in phase transformation and microstructure evolution. Directionally solidified, non-directionally solidified, quenched and specially heat treated alloys, relevant to the two peritectic reactions, L+NiAl->Ni2Al3 and L+Ni2Al3->NiAl3 in the Al-Ni model system, were investigated. A peritectic "reaction" is believed to occur instantly after a single nucleus of β forms on the primary phase α and result in a very thin peritectic rim, which may have different orientations. Generally, the primary phase α is mainly consumed during peritectic transformation and the amount of consumption may be defined as the "yield" of this step. It depends on the solid-state diffusion across the peritectic envelope and the composition relation between α and β. The diffusion, however, is hindered by the direct growth of β, which can become significant especially if β is located close to the peritectic liquid point and/or if the nucleation of β is difficult and the liquid is deeply undercooled. A new method is presented to tentatively predict the rate of a peritectic transformation according to phase diagram features, and it well accounts for the present experimental evidence that the transformation in L+NiAl->Ni2Al3 is extremely fast while that in L+Ni2Al3->NiAl3 extremely slow.

MM 45.3 Fri 11:00 IFW B

Homogeneous Nucleation and Crystal Crowth of Metallic Nanoparticle Superstructures — •Philip Born and Tobias Kraus — Leibniz-Institut for Neue Materialien (INM), Saarbrücken, Deutschland

The various interparticle interactions in nanoparticle suspensions lead to a phase diagram which is akin the thermodynamic phase diagram of atomic gases. In the atomic-gas-like state of colloidal suspensions, assembly is driven by the strength and directionality of the interparticle potentials, whose range is large compared to the particle size. The phase diagram alters drastically when the ratio between the particle size and the range of the interparticle forces increases. The liquid phase vanishes with increasing ratio, and the system eventually exhibits the temperature-independent jamming phase diagram of macroscopic granular media.

Here, we use sterically stabilized gold nanoparticles as a model system to explore experimentally the thermodynamic concentration-temperature (c-T) phase diagram of a colloidal suspension. We focus on the ordering of the emerging superstructures after quenching the system to the instable regime. By exchanging the capping layer of the gold particles the ratio between particle size and interaction potential range and the interactions among the ligand shells of particles can be changed. By systematically increasing the capping layer thickness, the transition from a rather atom-like to a granular media-like state can be observed. The interactions among the ligand shells of the particles change the interparticle friction and inhibit rearrangement.

MM 45.4 Fri 11:15 IFW B

Effect of production route on microstructural development during heat treatment of nanocrystalline NiTi and NiZr alloys — •Reeti Singh[1], Sergiy Divinski[1], Harald Rösner[1], Ruslan.Z Valiev[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wihelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149, Münster, Germany — [2]Institute of Physics of Advanced Materials, Ufa State Aviation University, 12 K. Marx Street, 450000 Ufa, Russian Federation

A comparative study of an amorphous NiTi alloy, produced by severe plastic deformation via high-pressure torsion (HPT) and a NiZr alloy, produced by HPT, repeated cold rolling (RCR) and melt-spinning (MS), is presented. The microstructure evolution is investigated in dependence on the production route by differential scanning calorimetry (DSC), X-ray diffraction analysis and transmission electron microscopy. The DSC signals observed during continuous heating experiments indicate a large separation between the crystallization and growth stages in the amorphous NiTi and NiZr alloys. A detailed analysis of the evolution of the enthalpy release revealed reproducibly non-monotonous trends with the annealing temperature that cannot be explained solely with nucleation and growth of crystalline volume fractions. However, these results as well as detailed kinetics analyses indicate that a reverse amorphization process occurred during annealing around 523 K in the NiTi alloy. The vitrification and crystallization characteristics of NiZr amorphized by HPT, RCR and MS are analyzed for comparison.

MM 45.5 Fri 11:30 IFW B

Laser-induced condensation in model colloid-polymer mixtures: ultralow interfacial free energies between coexisting phases — •Tim Neuhaus[1], Richard L C Vink[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institute of Theoretical Physics, Georg-August-Universität Göttingen, Germany

Laser-induced condensation occurs when a system with a bulk liquid-vapor transition is placed into a static external potential which is oscillating in one direction with a wavelength λ. The latter can be realized for colloidal particles by a standing laser field. It was shown previously [1], that for sufficiently large wavelengths λ, the bulk critical point splits into two critical points and a triple point with an intermediate "stacked fluid" phase which is partially condensed in sheets perpendicular to the oscillation direction. These results were obtained by using fundamental measure density functional theory for a colloid-polymer mixture within the Asakura-Oosawa model. Here, we use the same model and technique and calculate the interfacial free energy between all coexisting phases and compare the results with simulation data. We find that the "stacked fluid"-fluid and "stacked fluid"-vapor surface free energies are extremely small.

[1] I. Götze et al, Mol. Phys. **101**, 1651 (2003).

MM 46: Mechanical Properties III

Time: Friday 10:30–13:15 Location: IFW D

MM 46.1 Fri 10:30 IFW D

Appearance of dislocation mediated and orientation selective deformation twinning in a bimodally textured FeMnNiCr alloy — •David Geissler[1,2], Jens Freudenberger[1], Alexander Kauffmann[1,2], Maria Krautz[1,2], Jörg Eickemeyer[1], and Ludwig Schultz[1,2] — [1]IFW Dresden, PF 270116, 01171 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany

The deformation behaviour of low stacking fault energy (SFE) materials is of great interest to Fe-Mn based austenitic steel research. By comparing the microstructural and texture evolution with tensile stress-strain response of a Fe-24Mn-7Ni-8Cr (mass percent) alloy a slip-dominated deformation process and, at a later stage of deformation, twinning induced plasticity (TWIP) is observed. The annealed starting material exhibits a bimodal fiber texture and the occurrence of TWIP is texture sensitive, i.e. deformation twinning is only observable in grains of one texture component. Based on these experimental results, a model is presented, which reflects an orientational and configurational peculiarity of fcc stacking faults bound by two Shockley partials. With this model the onset point of twinning is reflected by the starting point of stacking fault growth, i.e. movement of the leading partial and stopping of the trailing partial. Calculations based on this model allow to compatibly describe the mechanical behaviour from tensile testing with respect to the microstructural evolution. Furthermore a reasonable SFE of 12.2 mJ per square meter can be extracted from the test data by application of the model assumptions.

MM 46.2 Fri 10:45 IFW D

Influence of Microstructure on Thermo-Mechanical Fatigue of Al Thin Films on Substrates — •Walther Heinz[1] and Gerhard Dehm[1,2] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben — [2]Department Materials Physics, Montanuniversität Leoben, Austria

The difference in thermal expansion coefficient between Al and Si can cause interconnect failure by thermo-mechanical fatigue in microelectronic devices subjected to repeated thermal cycling. In this study the influence of grain orientation on damage evolution of 0.2 - 2μm thick Al films on Si and alumina substrates is analyzed by local electron backscattered diffraction in a scanning electron microscope. The films are cycled between 100°C and 450°C up to 10.000 times. The investigations reveal that texture is a route to avoid thermo-mechanical fatigue damage by selecting a sharp (111) fibre texture. This can be explained by orientation dependent plasticity.

MM 46.3 Fri 11:00 IFW D

Low cycle fatigue of lead free solder joints — •Lars Schemmann, Andre Wedi, Dietmar Baither, and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Presently solders containing lead are banned from consumer electronics. Important alternatives are the Sn-Ag-Cu (SAC) solders and solders containing antimony . This work studies the isothermal low cycle fatigue properties of SAC solders and the SnSb(8) solder. For the experiments, model solder joints were produced and used. They consist of two pure copper plates joined together by a circular disk of solder. Low cycle fatigue experiments were done under displacement control. Furthermore hardness was tested by a micro indenter. In order to find an explanation for the different lifetimes of the solders, several micro structural investigations were performed. For this we used transmission and scanning electron microscopy as well as optical microscopy. The measured data showed a strong relation between lifetime and hardness of the solder alloy. We also found, that the type of solder influences the crack propagation.

MM 46.4 Fri 11:15 IFW D

Brittle-to-ductile transition of the intermetallic compound YCu — •Rolf Schaarschuch[1], Carl-Georg Oertel[1], Guanghui Cao[2], H.N. Tian[2], Jens Freudenberger[3], Heinz-Günter Brokmeier[4], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Materials Engineering, Shanghai University, Shanghai 200072, P.R. China — [3]Institute for Metallic Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [4]GKSS-Forschungszentrum Geesthacht GmbH, Max-Planck-Straße, 21494 Geesthacht, Germany

The temperature dependence of the tensile deformation behaviour of an extruded, polycrystalline YCu intermetallic compound with B2 structure at room temperature was investigated in the temperature range from room temperature down to 77K. The samples were deformed along the extrusion axis characterized by a weak <110>-fibre texture. The brittle-to-ductile transition (BDT) was found around 140K. The BDT is related to the transformation of the cubic B2 to the orthorhombic B27 structure proved by X-ray diffraction.

MM 46.5 Fri 11:30 IFW D

Intermediate temperature embrittlement in high purity nickel and binary nickel-bismuth alloy — •Lei Zheng[1,2], Reda Chellali[2], Dietmar Baiter[2], and Guido Schmitz[2] — [1]School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, 10083, China — [2]Institute of Materials physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149, Muenster, Germany

Intermediate temperature embrittlement (ITE) is a general phenomenon in Ni-based superalloys. Comparisons of existing interpretations given by different authors reveal considerable differences in understanding the mechanism of ITE. To clarify this situation, high purity nickel and binary Ni-Bi alloy were selected as the tested alloys and their tensile tests in the temperature range of room temperature to 850 °C were carried out. It was demonstrated clearly that high purity nickel has no ITE while Ni-Bi alloys show evident one. With the elevation in temperature, elongation after fracture decreases gradually to a minimum around 750 °C and then increases again rapidly. According to the experimental results, it must be concluded that the ITE is an impurity effect.

MM 46.6 Fri 11:45 IFW D

Deformation behaviour of cryo-drawn CuAl-wires — •Alexander Kauffmann[1,2], Jens Freudenberger[1], Yin Song[1,2], Tom Marr[1,2], Vadlamani Subramanya Sarma[3], Jürgen Eckert[1,2], and Ludwig Schultz[1,2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — [3]Dept. Metallurgical and Materials Engineering, IIT Madras, Chennai 600036, India

The effect of temperature on the active deformation mechanism is studied. For this purpose cryogenic drawing of several CuAl alloys was performed. Hence, a solid lubrification is needed which remains operating at cryogenic temperatures. We present a comparison of several solid lubricants for the deformation of two Copper alloys.

The comparison cryogenic temperature deformation of several CuAl alloys with conventionally drawn wires shows that the strengthening of these alloys during the deformation process is significantly affected by their stacking fault energy. The deformation at cryogenic temperature is most effective at intermediate stacking fault energies. This is interpreted in terms of a changing deformation mechanism from dislocation slip to deformation twinning. The analysis of the microstructure during the deformation process strengthens these assumptions.

MM 46.7 Fri 12:00 IFW D

Investigation of the mechanical properties of the 413-MAX phase Ti_4AlN_3 by perturbed γ-γ angular correlation — •Christoph Brüsewitz[1], Daniel Jürgens[1], Michael Uhrmacher[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 are nanolaminated layered carbides and nitrides, which feature an unusual set of the best attributes of both metals and high-performance ceramics. Due to their layered structure these phases are good electric and thermal conductors, superb thermal and mechanical shock resistant and easily machinable. To investigate the microscopic behaviour of these phases under uniaxial load, we selected Ti_4AlN_3 and performed measurements by using perturbed γ-γ angular correlation (PAC). The PAC method uses the oscillating anisotropy in the decay cascade of implanted ^{111}In, which is influenced via the hyperfine interaction by the local probe environment. The measured electric

field gradient (EFG) and especially the change of the frequency damping show the elasticity under applied and after released pressure in a sub-nanometer around the Al-site. Those measurements were not affected by the already known kink band formation in MAX phases under applied stresses, which are used to describe the high elasticity on the μm scale, as long as the phase is still stable. Therefore XRD was chosen to prove that the phase did not decompose. This work is supported by the DFG under contract HO 1125/19-1.

MM 46.8 Fri 12:15 IFW D

Influence of grain boundaries and crack length on the propagation of microstructurally short cracks in austenitic stainless steel — •Michael Scharnweber[1], Carl-Georg Oertel[1], Vladimir Mikulich[2], Wolfgang Tirschler[1], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, TU Dresden, 01062 Dresden — [2]Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, 09126 Chemnitz

Austenitic stainless steel (X2 CrNiMo 18 14 3) was cyclically deformed at RT in air under plastic strain control with amplitudes of 5×10^{-4} and 2×10^{-3}. Every 30.000 and 3.000 cycles, respectively, the samples were investigated in the scanning electron microscope in order to determine the propagation rate of the existing microstructurally short cracks as well as the corresponding distance between the crack tip and the opposing grain boundary. The results will be discussed with regard to the barrier effect of grain boundaries to crack propagation as well as the correlation between crack length and propagation rate at different strain amplitudes.

MM 46.9 Fri 12:30 IFW D

A phase-field study of crack propagation — •Daniel Schneider[1], Jan Höhn[1], Michael Selzer[1,2], Alexander Vondrous[2], Marcus Jainta[2], and Britta Nestler[1,2] — [1]Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology — [2]Institute of Materials and Processes, Karlsruhe University of Applied Science

An extension of the phase-field model is formulated incorporating a formulation for elastic and plastic effects on the evolution of microstructure. We show an approach to describe linear elasto-plastic and linear hardening material behavior based on the Prandtl-Reuss model in the context of the phase-field method. Adapted boundary conditions for the different field quantities allow a more accurate modeling of experimental processes. We validate the simulations by a comparison of stress profiles with analytically predicted stress fields of brittle fracture and with the energy criterion according to Griffith theory. Further we present simulations of micro crack propagation induced by external stresses in both, two phase systems as well as polycrystalline structures. The dynamics of the crack formation and the shape of the phase boundaries are analyzed for different processing conditions.

MM 46.10 Fri 12:45 IFW D

Fracture as Pattern Formation Process — •Robert Spatschek[1], Michael Fleck[2], Denis Pilipenko[2], and Efim Brener[3] — [1]Max-Planck-Institut für Eisenforschung — [2]Universität Bayreuth — [3]Forschungszentrum Jülich

Fracture is an important process in materials science, that still lacks fundamental understanding. Here we report on a series of theoretical investigations and numerical simulations on crack propagation, which treat this problem in the spirit of an interfacial pattern formation process. This means, that not only the crack velocity, but also the entire shape of the crack with a finite tip radius is self-consistently predicted by the theory. For fast cracks in brittle materials with velocities close to the speed of sound inertial effects become important, and for lower speeds, in particular close to the Griffith point, we consider viscoelastic bulk dissipation as efficient selection mechanism for steady state crack growth. We use phase field simulations to describe also the combined effect of both inertia and bulk damping. Alternatively, multipole expansion methods provide exact solutions for each effect separately, and perturbative approaches are used for the combination of both physical effects. Altogether, this allows to obtain a broad perspective on the predictions of the crack growth models.

MM 46.11 Fri 13:00 IFW D

Ab-initio calculation of second- and third-order elastic constants — •Rostam Golesorkhtabar[1,2], Pasquale Pavone[1,2], Jürgen Spitaler[1,2], Peter Puschnig[1], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Forschung Gmbh, Austria

Elastic properties of solids play a key role in materials science and technology. Various mechanical and thermodynamical properties are directly connected to elastic constants of different orders. In particular, the analysis of nonlinear quantities such as the third-order elastic constants (TOEC) gives a direct way of exploring the effect of anharmonicity of the lattice potential. In this work, we present a framework for the first-principles calculation of both second-order elastic constants (SOEC) and TOEC. We have implemented their calculation in the `ElaStic` package. The latter is now able to evaluate the full SOEC and TOEC for any crystal structure from ab-initio total-energy and/or stress calculations. We have applied `ElaStic` to obtain SOEC for one representative crystal of the 9 different symmetry classes. Furthermore, we calculate the TOEC and pressure dependence of the SOEC for diamond, hexagonal Mg, and rhombohedral Al_2O_3. The calculations are performed using total energy and stress data from the FP-LAPW codes WIEN2k and `exciting` and the pseudo-potential code Quantum ESPRESSO. Our results demonstrate the `ElaStic` describes with high precision linear and nonlinear elastic constants for materials characterized by different chemical bonding.