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Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks (Hauptvorträge) and Sessions

(lecture rooms TC 006, H 0106, H 0107, H 1029; Poster B)

Invited Talks (Hauptvorträge)

MM 1.1	Mon	9:30–10:00	H 0107	**Production of Multifunctional Materials Using High-Pressure Torsion** — •Zenji Horita
MM 10.1	Mon	15:00–15:30	H 0107	**Microstructural and mechanical anisotropy of ultra fine grained metals and alloys after ECAP** — •Martin Wagner, Matthias Hockauf
MM 18.1	Tue	9:30–10:00	H 0107	**Twinning-mediated plasticity in Au Nanowires** — Andreas Sedlmayr, Reiner Mönig, Gunther Richter, •Oliver Kraft
MM 27.1	Wed	9:30–10:00	TC 006	**First-principles Predictions of Solute Strengthening in Al and Mg alloys** — •William Curtin, Gerard Leyson
MM 42.1	Wed	18:00–18:30	H 0107	**In-situ Transmission Electron Microscopy of Phase Transformations in Materials** — •Erdmann Spiecker
MM 43.1	Wed	18:30–19:00	H 0107	**Advancing ab initio methods to finite temperatures for applications in materials design** — •Tilmann Hickel, Alexey Dick, Fritz Körmann, Blazej Grabowski, Jörg Neugebauer
MM 44.1	Thu	9:30–10:00	H 0107	**Positrons Probing Matter: Bulk and Thin Film Studies Using the Low-Energy Positron Beam at NEPOMUC** — •Chrisotph Hugenschmidt
MM 52.1	Thu	15:00–15:30	H 0107	**A renaissance in atom-probe tomography for the study of all materials** — •David Seidman

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H 0107	**HV Horita**
MM 2.1–2.6	Mon	10:15–11:45	TC 006	**Computational Materials Modelling I - Multiscale: Fundamentals**
MM 3.1–3.5	Mon	10:15–11:45	H 0107	**Topical Session Bulk Nanostrucured Materials I - Processing**
MM 4.1–4.5	Mon	10:15–11:30	H 0106	**Mechanical Properties I**
MM 5.1–5.5	Mon	10:15–11:30	H 1029	**Transport and Diffusion I**
MM 6.1–6.5	Mon	11:30–12:45	H 0106	**Mechanical Properties II**
MM 7.1–7.5	Mon	11:30–12:45	H 1029	**Transport and Diffusion II**
MM 8.1–8.5	Mon	11:45–13:00	TC 006	**Computational Materials Modelling II - Methods**
MM 9.1–9.4	Mon	11:45–13:00	H 0107	**Topical Session Bulk Nanostrucured Materials II - Processing**
MM 10.1–10.1	Mon	15:00–15:30	H 0107	**HV Wagner**
MM 11.1–11.5	Mon	15:00–17:45	EB 202	**Joint Session FePt Nanoparticles (jointly with DS, MM)**
MM 12.1–12.5	Mon	15:00–17:30	H 0105	**Joint Symposium 100 years of X-ray diffraction: from the Laue experiment to new frontiers (jointly with KR, BP, CPP, DF, MA, MM, GP)**
MM 13.1–13.5	Mon	15:45–17:00	TC 006	**Computational Materials Modelling III - Alloys**
MM 14.1–14.6	Mon	15:45–17:15	H 0107	**Topical Session Bulk Nanostrucured Materials III - Microstructure and Characterization I**
MM 15.1–15.5	Mon	15:45–17:00	H 0106	**Mechanical Properties III**
MM 16.1–16.5	Mon	15:45–17:00	H 1029	**Microstructure and Phase Transformations I**

MM 17.1–17.89	Mon	17:00–19:00	Poster B	**Poster Session**
MM 18.1–18.1	Tue	9:30–10:00	H 0107	**HV Kraft**
MM 19.1–19.7	Tue	10:15–12:00	TC 006	**Computational Materials Modelling IV - Finite Temperature**
MM 20.1–20.4	Tue	10:15–11:30	H 0107	**Topical Session Bulk Nanostrucured Materials IV - Microstructure and Characterization II**
MM 21.1–21.6	Tue	10:15–11:45	H 0106	**Microstructure and Phase Transformations II**
MM 22.1–22.5	Tue	10:15–11:30	H 1029	**Functional Materials I**
MM 23.1–23.6	Tue	11:30–13:00	H 0107	**Topical Session Bulk Nanostrucured Materials V - Microstructure and Characterization III**
MM 24.1–24.4	Tue	11:30–12:30	H 1029	**Functional Materials II**
MM 25.1–25.5	Tue	11:45–13:00	H 0106	**Microstructure and Phase Transformations III**
MM 26.1–26.4	Tue	12:00–13:00	TC 006	**Computational Materials Modelling V - Fracture and Other Failure Mechanisms**
MM 27.1–27.1	Wed	9:30–10:00	TC 006	**HV Curtin**
MM 28.1–28.4	Wed	10:15–11:30	TC 006	**Topical Session Theory meets Experiment I - Intermetallics and Steels**
MM 29.1–29.5	Wed	10:15–11:45	H 0107	**Topical Session Bulk Nanostrucured Materials VI - Mechanical Properties I**
MM 30.1–30.5	Wed	10:15–11:30	H 0106	**Functional Materials III**
MM 31.1–31.8	Wed	10:15–12:15	H 1029	**Nanocharacterization**
MM 32.1–32.4	Wed	11:30–12:30	H 0106	**Functional Materials IV**
MM 33.1–33.5	Wed	11:30–13:00	TC 006	**Topical Session Theory meets Experiment II - Nanocomposites and Microstructure**
MM 34.1–34.5	Wed	11:45–13:00	H 0107	**Topical Session Bulk Nanostrucured Materials VII - Mechanical Properties II**
MM 35.1–35.4	Wed	15:00–16:15	TC 006	**Topical Session Theory meets Experiment III - Bond-order Potentials and Finite Temperature**
MM 36.1–36.5	Wed	15:00–16:30	H 0106	**Topical Session Bulk Nanostrucured Materials VIII - Functional Properties I**
MM 37.1–37.5	Wed	15:00–16:45	H 0107	**Topical Session Modern Atom Probe Tomography I - Fundamentals**
MM 38.1–38.8	Wed	15:00–17:00	H 1029	**Liquid and Amorphous Metals**
MM 39.1–39.5	Wed	16:15–17:45	TC 006	**Topical Session Theory meets Experiment IV - Batteries, Thermoelectrics and Thermal Barrier Coatings**
MM 40.1–40.5	Wed	16:30–17:45	H 0106	**Topical Session Bulk Nanostrucured Materials IX - Functional Properties II**
MM 41.1–41.4	Wed	16:45–17:45	H 0107	**Topical Session Modern Atom Probe Tomography II - Functional Materials**
MM 42.1–42.1	Wed	18:00–18:30	H 0107	**HV Spiecker**
MM 43.1–43.1	Wed	18:30–19:00	H 0107	**HV Hickel**
MM 44.1–44.1	Thu	9:30–10:00	H 0107	**HV Hugenschmidt**
MM 45.1–45.6	Thu	10:15–11:45	TC 006	**Computational Materials Modelling VI - Thermal Conductivity and Transport**
MM 46.1–46.6	Thu	10:15–11:45	H 1029	**Nanomaterials I**
MM 47.1–47.5	Thu	10:15–11:45	H 0107	**Topical Session Modern Atom Probe Tomography III - Functional and Nanostructured Materials**
MM 48.1–48.7	Thu	10:15–12:00	H 0106	**Joint Session Magnetic Shape Memory Alloys I (jointly with DS, MA)**
MM 49.1–49.5	Thu	11:45–13:00	H 1029	**Nanomaterials II**
MM 50.1–50.5	Thu	11:45–13:00	H 0107	**Topical Session Modern Atom Probe Tomography IV - Thin Films and Structural Materials**
MM 51.1–51.5	Thu	11:45–13:00	TC 006	**Computational Materials Modelling VII - Oxides**
MM 52.1–52.1	Thu	15:00–15:30	H 0107	**HV Seidman**
MM 53.1–53.14	Thu	15:00–18:45	H 0112	**Joint Session Magnetic Shape Memory Alloys II (jointly with DS, MA)**
MM 54.1–54.6	Thu	15:45–17:15	TC 006	**Computational Materials Modelling VIII - Mechanical Properties and Strain**
MM 55.1–55.5	Thu	15:45–17:00	H 0107	**Topical Session Modern Atom Probe Tomography V - Steels, Alloys and Structural Materials**
MM 56.1–56.4	Thu	15:45–16:45	H 0106	**Biomaterials**
MM 57.1–57.5	Thu	15:45–17:00	H 1029	**Complex Materials I**

MM 58.1–58.4	Thu	17:00–18:00	H 0107	**Topical Session Modern Atom Probe Tomography VI - Ordering, Clustering and Segregation**
MM 59.1–59.5	Thu	17:00–18:15	H 1029	**Complex Materials II**
MM 60.1–60.7	Thu	17:15–19:00	TC 006	**Computational Materials Modelling IX - Interfaces and Boundaries**

Topical session "Modern Atom Probe Tomography"

Organizers: Prof. Dr. Guido Schmitz (Universität Münster), Prof. Dr. Cynthia Volkert (Universität Göttingen), Prof. Dr. Dierk Raabe (MPIE Düsseldorf)
Atom probe tomography has experienced tremendous progress by introduction of laser pulsing and efficient wide-angle detector systems. Nowadays, the method represents a versatile tool of nano-analysis that can be applied not only to complex metallic alloys but also ceramics, semi-conductors and even polymeric and biomaterials. An increasing number of instruments are presently installed in many laboratories in Germany and Europe. To reflect this exciting development, the symposium invites all kinds of contributions addressing recent methodic aspects as well as examples of applications. Reports on latest instrumentation, physics of high field laser-matter interaction, tomographic data reconstruction are highly welcome as well as current studies by atom probe tomography on chemical structure and solid state reactions in nanostructured materials, in alloys and various functional materials. Also, presentations involving both, atom probe tomography and directly related kinetic-thermodynamic simulations are welcome.

Topical session "Bulk Nanostructured Materials"

Organizers: Prof. Dr. Roland Würschum (Technische Universität Graz), Prof. Dr. Gerhard Wilde (Universität Münster), Prof. Dr. Mathias Göken (Universität Erlangen-Nürnberg)
Research and development in the field of bulk nanostructured materials has become a prominent topic in modern materials science over the last years. Severe plastic deformation (SPD), in particular by high-pressure torsion (HPT), equal channel angular processing (ECAP), or accumulative roll bonding (ARB), is currently seen as the most prospective processing route for the synthesis of bulk nanophase metals. In addition to the inherent large-scale size, attractive mechanical properties such as high strength in combination with good ductility are associated with the pore-free ultra-fine grained structure of SPD-processed metals. Most recently, also functional properties of bulk nanostructured materials have increasingly moved into the focus, reaching from SPD-processed nanocrystalline magnetic alloys or bulk shape memory nanoalloys to nanometals and alloys for hydrogen storage as well as to thermoelectric materials.
The topical session intends to provide a forum for scientific exchange in this interdisciplinary field of bulk nanostructured materials. Oral and poster presentations on synthesis, structure, and properties of these fascinating new materials, including theory and modelling, are highly welcome.

Topical session "Materials Design on the Atomistic Scale: Theory meets Experiment"

Organizers: Prof. Dr. Jörg Neugebauer (MPIE Düsseldorf), Prof. Dr. Reiner Kirchheim (Universität Göttingen)
Thanks to impressive new developments and techniques both in theory and experiment enormous progress has been made in characterizing and understanding materials on the atomistic scale. Theoretical simulations made huge progress, both with respect to predictive power and complexity of structures and questions that can be addressed. Advances in electron microscopy, 3D atom probe, synchrotron radiation, neutron scattering, or scanning tunneling microscopy to name only a few allow nowadays a spatial and temporal resolution unimaginable a few years ago. These advances in theory and experiment open a new and exciting interdisciplinary field with great opportunities for understanding and designing materials for next generation technological challenges. The aim of the symposium is to give a brief overview about recent achievements, new approaches and successful applications in the various fields and to provide a joint platform for the various scientific communities.

Invited talks of the Joint Symposium SYTM (MA, MM, DS) "Tailoring magnetism in $L1_0$-ordered nanostructures: Perspectives for magnetic recording beyond 1 Terabit/in^2"

See SYTM for the full program of the symposium.

SYTM 1.1	Mon	9:30–10:00	H 0105	**Thermally Assisted Magnetic Recording at 620 Gb/in^2 using Granular $L1_0$ FeCuPtAg-X Media** — •D. Weller, O. Mosendz, S. Pisana, T. Santos, G. Parker, J. Reiner, B. C. Stipe
SYTM 1.2	Mon	10:00–10:30	H 0105	**Large-area hard magnetic $L1_0$-FePt and composite $L1_0$-FePt based nanopatterns** — •Dagmar Goll, Thomas Bublat
SYTM 1.3	Mon	10:30–11:00	H 0105	**Electric field control of magnetic exchange coupling in FePt / Fe-O thin fims** — •Karin Leistner

SYTM 1.4	Mon	11:00–11:30	H 0105	**FePt-based exchange coupled composite media** — •Manfred Albrecht
SYTM 1.5	Mon	11:30–12:00	H 0105	**Optimization of FePt films for recording applications by micromagnetic modeling** — •Josef Fidler, Jehyun Lee, Barbara Dymerska, Dieter Suess

Invited talks of the Joint Symposium SYXD (KR, BP, CPP, DF, GP, MA, MI, MM) "100 years since the Laue experiment: Topical aspects of diffraction and scattering"

See SYXD for the full program of the symposium.

SYXD 1.1	Mon	15:00–15:30	H 0105	**Disputed discovery: The beginnings of X-ray diffraction in crystals** — •Michael Eckert
SYXD 1.2	Mon	15:30–16:00	H 0105	**Why are quasicrystals quasiperiodic?** — •Walter Steurer
SYXD 1.3	Mon	16:00–16:30	H 0105	**Coherent Diffraction Imaging with Free-Eletron Lasers** — •Massimo Altarelli
SYXD 1.4	Mon	16:30–17:00	H 0105	**X-ray free-electron lasers - emerging opportunities for structural biology** — •Ilme Schlichting
SYXD 1.5	Mon	17:00–17:30	H 0105	**Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling** — •Tim Salditt

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:30–20:30 Raum H 0107

This year's general meeting of the Metal and Materials Physics Division (FV MM) is taking place on Wednesday at 19:30 in room H 0107 after the invited talks (Hauptvorträge) by E. Spiecker and T. Hickel and the following social gathering. The meeting will be opened with a short welcome address and the report of the chairman of the Metal and Materials Physics Division (AGMM). Afterwards, all attendees are invited to suggest symposia and speakers which could be invited for the next spring meeting 2013 in Regensburg. Everybody is highly welcome to join the social gathering and participate at the annual meeting directly afterwards.

MM 1: HV Horita

Time: Monday 9:30–10:00 Location: H 0107

Invited Talk MM 1.1 Mon 9:30 H 0107

Production of Multifunctional Materials Using High-Pressure Torsion — •Zenji Horita — Kyushu University, Fukuoka, Japan

High-pressure torsion (HPT) is a processing procedure to introduce intense strain under high pressure. It is capable of refining the grain size to the submicrometer or nanometer range in bulk forms of metallic materials. Second phase particles in the metal matrix can be fragmented to a fine dispersion of nanosized particles or even dissolution of the particles may occur by severe plastic deformation during HPT processing. It is also possible to consolidate powders at relatively low temperatures so that alloying is attained through solid-state reaction and fabrication of metal-matrix composites is feasible without successive sintering process. Nanostructure control is further achieved through subsequent combination of annealing or aging process. This presentation shows that HPT can produce materials exhibiting multifunctionality with not only better mechanical properties but also additional functional properties improved in hydrogen storage capability, thermoelectric properties, electronic and magnetic properties, corrosion resistance and so on. Some examples are introduced from our recent studies using the HPT process.

MM 2: Computational Materials Modelling I - Multiscale: Fundamentals

Time: Monday 10:15–11:45 Location: TC 006

MM 2.1 Mon 10:15 TC 006

FHI-aims becomes embedded: full-potential QM/MM-approach — •Daniel Berger[1], Volker Blum[2], and Karsten Reuter[1] — [1]TU München — [2]Fritz-Haber Institut der MPG

Photoelectrochemical processes like water splitting add to the wide range of applications for which a computationally most efficient description of (possibly locally charged) semiconducting systems is required. Properly accounting for long-range electrostatics without getting troubled with spurious interactions with periodic images, embedded cluster models are an appealing option to this end. Here, we present a corresponding implementation for the full-potential FHI-aims package [1]. In order to prevent electron leakage into the Coulomb singularities, we describe the linking atoms at the QM/MM-boundary at the level of norm-conserving pseudopotentials. The fully non-local form of the employed Kleinman-Bylander pseudopotentials allows for fast evaluation of the interaction integrals, especially in combination with FHI-aims' efficient atom-centered basis sets. We demonstrate the high accuracy and computational efficiency of this approach with applications to TiO_2(110)-supported metal clusters.

[1] V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175 (2009).

MM 2.2 Mon 10:30 TC 006

Atomistic and continuum regions: Effects of coupling — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Molecular dynamics simulations are a standard technique in computational materials modelling. The size of investigated solid structures, however, is limited to about the micrometer length scale. Finite element methods are less restricted in this respect but lack the atomistic description of matter. Obviously, this leads to the idea to couple both methods. The region of interest then is treated in an atomistic fashion and connected to a linear elastic continuum outside.

In this talk, fundamental effects are presented that arise in dynamic multiscale hybrid simulations due to the interface region. The scheme and procedures are illustrated, which are required to connect the two methods. In a simple setup aluminium has been chosen as a test case. In the numerical experiments, one domain determines the displacement boundary conditions for the other. The results show that the corresponding fixed boundaries influence relaxation. The decomposition into two parts also leads to a sort of asynchronism in time. In the case of strong excitations, it is observed that the anharmonic contributions lead to a deviation from linear elasticity, which is used in the continuum. Furthermore, depending on the spatial resolution of the FE mesh, short-wavelength phonons are reflected backwards into the atomistic domain.

MM 2.3 Mon 10:45 TC 006

A Two Scale Approach to Model the Freeze Casting Process — •Frank Wendler[1,2], Marcel Huber[2], and Britta Nestler[1,2] — [1]IMP, Karlsruhe University of Applied Sciences, Karlsruhe — [2]IAM-ZBS, Karlsruhe Institute of Technology, Karlsruhe

In the last years the freeze casting process has been adapted to a broad variety of materials with open porosities between 10 and 90 % (ceramics, polymers, metals). The crystallization kinetics of ice into an aquaeous colloidal suspension leads to the rejection of dispersed ceramic particles from the growing ice front and results in complex lamellar patterns, commonly explained by a Mullins-Sekerka instability of the constitutionally supercooled ice-colloid interface.

For a quantitative prediction of macro- and microscopic process variables (freezing conditions, solid fraction, particle size, colloidal interaction) on the microstructure, we simulate the free boundary problem using a multi phase-field model based on a thermodynamic free energy formulation on two different length scales: At the particle scale (50 μm) the inert particles are resolved and interact with each other and the ice front. We briefly show how the model parameters (interface tensions + mobilities, higher order potential, interface width) represent capillary properties of the colloid. At a large scale (1000 μm) the osmotic pressure of the colloid as a function of the solid particle fraction is integrated into the free energy formulation, from which diffusion coefficients are derived. We determine the limiting velocities for particle pushing and the transition from lamellar to isotropic growth from simulations, and compare them to an experimental system (ZrO2/water).

MM 2.4 Mon 11:00 TC 006

Molecular Dynamics Simulations of Laser Ablation in Metals: Parmeter Dependence, Double Pulses, and Extended Models — •Johannes Roth, Johannes Karlin, Marc Sartison, Armin Krauss, and Hans-Rainer Trebin — ITAP, Universität Stuttgart

Femtosecond laser ablation of metals depends on three parameters: electron heat conductivity, electron heat capacity and electron-phonon coupling. With respect to these parameters all metals can be devided into classes. Keeping the interaction and the crystal structure fixed we have varied the parameters within the experimentally observed range. We find that the heat capacity plays a minor role whereas the other parameters are equally important.

In a second part we have studied the melting behavior and ablation properties of Al under the influence of non-Gaussian and double pulses at a certain time interval. In general we find that a simple Gaussian pulse is the most effective method to ablate material.

The ablation by femtosecond laser pulses is a process dominated by the free electrons of the metal. To model the process correctly, one uses the two-temperature-model (TTM) with separete temperatures for the electrons and the lattice. The model still neglects a finite electron relaxation which is treated in an extended TTM. We show numerically and by simulations that the simple TTM leads to satisfactory results for Al and Nb, but that the extended TTM should be applied for example for Cu or Pb.

MM 2.5 Mon 11:15 TC 006

Computing Raman and infrared frequencies of nanostructures — •Felix Zörgiebel[1], Jens Kunstmann[1], Daijiro Nozaki[1], and Gianaurelio Cuniberti[1,2] — [1]Insitute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Division of IT Convergence Engineering and National Center for Nanomaterials Technology, POSTECH, Pohang 790-784, Republic of Korea

We developed a method to compute Raman and Infrared frequencies of nanostructures of arbitrary dimension. Our method is based on molecular dynamics simulations and a symmetry analysis of the structure of interest. The calculation of electric properties like the polarizability and dipole moment is not required, which makes our method usable with existing molecular dynamics software. Raman peak shifts for bulk silicon were calculated for different temperatures and lattice constants and showed good agreement with experimental observations. Additionally we calculated the dependence of the Raman peak shift of silicon nanowires on the wire diameter and on surface stress.

MM 2.6 Mon 11:30 TC 006

Fast, stable convergence of electronic structure calculations for nanomaterials — •Philip Hasnip — University of York, York, UK

Ab initio materials modelling methods have become essential tools for condensed matter physicists in a wide variety of fields. The advent of more and more powerful computers has allowed larger, more complex systems to be simulated and the dramatic improvements in both experimental growth and characterisation methods have allowed the length scale of theoretical simulations and experimental studies to coincide at the nanoscale.

Whilst there has been undoubted success in the modelling of nanostructures and materials, the approach is not without its problems. As the size of the simulation system is increased to the nanoscale, the conventional algorithms used to find the electronic groundstate often show poor convergence, and for large or complex systems they may fail to converge at all. We first discuss the root cause of these problems, and then present an alternative algorithm which is not only robust, but also faster for nanomaterials simulation.

MM 3: Topical Session Bulk Nanostrucured Materials I - Processing

Time: Monday 10:15–11:45 Location: H 0107

Topical Talk MM 3.1 Mon 10:15 H 0107

Generation of nanocomposites and super saturated solid solutions by SPD — •Reinhard Pippan, Andrea Bachmaier, Anton Hohenwarter, and Georg Rathmayr — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstr.12,

Severe plastic deformation (SPD) is a very powerful tool to generate ultrafine grained or nanocrystalline materials. The thermal stability of the SPD processed single phase materials is often low and the refinement is often limited to the 100 nm regime. In order to overcome this drawback we have tried to stabilize the grain structure and to generate even finer nanostructures by second phases. Different types of materials, composites of miscible and immiscible metals, dual phase metallic materials, metal-oxide composites with extreme variations in size and concentration of oxides have been HPT deformed up to very high strains. The microstructural evolution has been examined and the refinement process is analysed. In most cases a bulk nanocomposite or a supersaturated solid solution with nanocrystalline structure or a mixture of them is formed. The fragmentation process as well as the phenomena resulting in a supersaturated solid solution and finally in a saturation will be discussed. Finally, the stability of the different nanostructured is examined and the coarsening phenomena will be considered. Financial support by the FWF Austrian Science Fund is appreciated (project S 10402-N16).

MM 3.2 Mon 10:45 H 0107

The influence of total strain and deformation rate during the ECAP process on the microstructure, microhardness and kinetic properties of nickel — •Gerrit Reglitz[1], Sergiy Divinski[1], Harald Rösner[1], Vladimir Popov[2], Evgeniy Shorokhov[3], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Metal Physics, Russian Academy of Sciences, Ekaterinburg, Russia — [3]All-Russia Research Institute of Technical Physics, Russian Federal Nuclear Center, Snezhinsk, Russia

In the last years ultra-fine grained (UFG) materials produced by severe plastic deformation like equal channel angular pressing (ECAP) or high-pressure torsion became an intensive research topic due to the improved properties which these highly deformed materials offer.

By ECAP it is possible to produce materials with different microstructures through changing the process parameters such as the total introduced strain, the deformation rate or the deformation temperature. In this work the total strain was varied by using different numbers of ECAP passes between 2 and 12, while the deformation rate was varied from 10^{-2} s^{-1} (standard ECAP) to 10^{4} s^{-1} (explosive ECAP). The microstructure, microhardness and the kinetic properties of grain boundaries in the different materials are investigated and comparatively discussed.

Support by DFG is gratefully acknowledged.

MM 3.3 Mon 11:00 H 0107

Cu(Bi) alloys processed by Dynamic plastic deformation — •Henning Edelhoff[1], Harald Rösner[1], Matthias Wegner[1], Boris Straumal[2], Zhenbo Wang[3], Ke Lu[3], Sergij Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Russia — [3]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, China

Due to the increased interest in improved materials properties by microstructural refinement numerous synthetic techniques have been developed. One special method of plastic deformation, is the so-called dynamic plastic deformation (DPD) conducted at cryogenic temperatures and high strain rates leading to nanostructured materials. In the case of pure copper, alongside to grain refinement, an increasing tendency of deformation twinning is observed [1]. In this work, the DPD technique is used to deform copper-bismuth alloys with 200 and 1200 ppm bismuth, respectively. The ultrafine grained samples produced by DPD were examined by means of X-ray diffraction analysis, transmission electron microscopy and scanning electron microscopy combined with electron back scatter diffraction. The influence of bismuth on the microstructural refinement was investigated, following a special interest in segregation of bismuth at deformation twin boundaries.

[1] Y.S. Li, N.R. Tao, K. Lu, Acta Mater, 56, 230 (2008)

MM 3.4 Mon 11:15 H 0107

Comparison of the saturation structures of intermetallic alloys subjected to severe plastic deformation — •Christian Rentenberger, Christoph Gammer, David Geist, and Hans-Peter Karnthaler — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria.

Microstructural refinement by severe plastic deformation is a method to achieve novel mechanical properties. Considerable attention has been devoted to pure metals and solid solution alloys but only a few studies have been carried out on intermetallic alloys. The main reason is their high brittleness making them difficult to deform. In the present work based on transmission electron microscopy (TEM) investigations the saturation structures yielded by high pressure torsion deformation of different intermetallic compounds are compared: Ni_3Al ($L1_2$ ordered), Zr_3Al ($L1_2$ ordered) and FeAl (B2 ordered). The structures are studied in three dimensions by using both different sections and novel TEM methods [1]. It is concluded that depending on the type of lattice defects induced by deformation different saturation structures are occurring: a nanocrystalline structure showing the loss of chemical long-range order or an amorphous one with residual nanograins [2,3].

[1] C. Gammer, C. Mangler, H. P. Karnthaler, C. Rentenberger. Micr. Microanal. 17, 866 (2011). [2] C. Mangler, C. Gammer, H. P. Karnthaler, C. Rentenberger, Acta Mater. 58, 5631 (2010). [3] D. Geist, C. Gammer, C. Mangler, C. Rentenberger, H. P. Karnthaler. Phil. Mag. 90, 4635 (2010). This work was supported by the Austrian Science Fund (FWF): [S10403, P22440].

MM 3.5 Mon 11:30 H 0107

Effect of hydrostatic pressure on the microstructure and mechanical properties during and after high pressure torsion — •Erhard Schafler, Roman Schuster, Michael Kerber, and Florian Spieckermann — Universität Wien, Fakultät für Physik, Physik Nanostrukturierter Materialien

The hydrostatic pressure is a general feature of severe plastic deformation (SPD) methods, especially when performing high pressure torsion

(HPT). It is essential for achieving the high strains and to introduce the high amount of lattice defects, which are necessary for the fragmentation into an ultra-fine grained materieal. The investigations of HPT-processed Cu and Ni under variation of the hydrostatic pressure revealed marked differences between the in-situ torsional stress (torque measurement) and the post-HPT flow stress of the ultrafine-grained materials. A special experimental procedure was designed to simulate the hydrostatic pressure release, in order to gain insight into the processes behind unloading. Investigations by X-ray line profile analysis and hardness measurement show marked influences of the pressure release on microstructure and strength. While the size of the coherently scattering domains indicate that the fragmentation process is already finished during the HPT-deformation, the dislocation density decreases drastically and the arrangement of the dislocations within the subgrain structure changes to a less stress-intensive one, upon pressure release. In parallel the hardness decreases significantly and confirms the discrepancy between in-situ torque-stress and post-HPT flow stress. Work supported by the Austrian Science Fund, project S 10403

MM 4: Mechanical Properties I

Time: Monday 10:15–11:30 Location: H 0106

MM 4.1 Mon 10:15 H 0106

In-situ TEM mechanical testing of nanocrystalline Cu — •Matthias Funk[1], Claiare Chisholm[3], Anna Castrup[2], Daniel Kiener[4], Andrew Minor[3], and Christoph Eberl[1] — [1]KIT, Institute for Applied Materials, Kaiserstrasse 12, 76131 Karlsruhe, Germany — [2]KIT, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]Department of Materials Science and Engineering, University of California, Berkeley, USA — [4]Austrian Academy of Science, Erich Schmid Insitute of Materials Science, Jahnstrasse 12, 8700 Leoben, Austria

For nanocrystalline (nc) materials deformation seems to be governed by processes at the grain boundaries. Therefore, it is necessary to observe the microstructural changes during deformation to fully understand the mechanisms involved. In-situ TEM tensile and cycling tests were conducted on sputtered nc Cu thin films with a thickness of 60 nm. The sputtered films were transferred onto a Push-to-Pull device to test it with an in situ Picoindenter. The continuous films were milled into an hour glass shape by the use of a FIB tool with a gage width and length of roughly 3 and 4 um. Videos were taken of the single cycles in combination with micrographs at the end of each cycle. The strain of up to 9% was analyzed with digital image correlation globally over the whole sample as well as locally. The ultimate tensile strength reached 2 GPa and the Youngs modulus round about 50 GPa. During cycling, grain coarsening was observed. The high observed strength and ductility will be discussed in the light of the microstructural changes during tensile and fatigue testing and the small testing volume.

MM 4.2 Mon 10:30 H 0106

Strain Relaxation Kinetics in Thin Nano-Crystalline Platinum Films — •Wolfgang Gruber[1], Carsten Baehtz[2], Christian Kübel[3], Wolfram Leitenberger[4], and Harald Schmidt[1] — [1]TU Clausthal, Institut für Metallurgie — [2]Helmholtz Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research — [3]Karlsruher Institut für Technologie, Karlsruher Micro Nano Facility — [4]Universität Potsdam, Institut für Physik und Astronomie

Thin metal films with a thickness in the nanometer to the micrometer range are important for various areas of science and technology. Residual stresses, which are commonly assumed to be bi-axial in thin films, result from different thermal expansion coefficients of substrate and film (thermal stress) and/or from stress formation during film deposition (grown-in stress). During isothermal annealing, residual stresses relax as a function of annealing time and temperature. We used thin nano-crystalline Pt films deposited on oxidized silicon wafers to investigate the role of vacancies for relaxation of strain resulting from compressive stress. We applied a method which is based on the fundamental concept of dilatometry. We modified this basic concept and used synchrotron based combined in-situ X-ray diffractometry and reflectometry. From the experimentally determined relative changes of the lattice parameter and of the film thickness the modification of vacancy concentration and residual strain was derived as a function of annealing time. The results indicate that relaxation of strain is accompanied by the creation of vacancies at the free film surface [1].

[1] W. Gruber et al., Phys. Rev. Lett., in print.

MM 4.3 Mon 10:45 H 0106

Accumulative roll bonding and differential speed rolling of ultra fine grained Al-Ti composites — •Jan Romberg[1,2,3], Juliane Scharnweber[4], Jens Freudenberger[1,5], Hiroyuki Watanabe[6], Tom Marr[1,2], Carl-Georg Oetrel[4], Werner Skrotzki[4], and Ludwig Schultz[1,2] — [1]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]Dresden University of Technology, Institute for Materials Science — [3]Dresden University of Technology, ECEMP International Graduate School, Germany — [4]Dresden University of Technology, Instute for Solid State Physics — [5]Freiberg University of Technology, Institute of Materials Science, Freiberg, Germany — [6]Osaka Munipial Technical Research Institute, Osaka, Freiberg

Roll bonding of aluminium and titanium sheets was performed accumulatively. Due to the differences in formability of the metals initially used necking of the titanium is observed. Hence this process would not be expected to generate sheets consisting of layers from titanium and aluminium with a homogeneous thickness. This study examines the conditions under which roll bonding of titanium and aluminium is feasible and how necking can be suppressed. The use of cold worked aluminium sheets and recrystallised titanium sheets enables accummulated roll bonding with up to four cycles and faultless deformation. In addition the potential of differential speed rolling with respect to increasing the ductility of the roll bonded metals is shown. Both processes were combined to assess the relationship between processing and properties of fine-grained laminar sheets from titanium and aluminium.

MM 4.4 Mon 11:00 H 0106

The new Shock-Wave-Laboratory at the TU Bergakademie Freiberg — •Thomas Schlothauer[1], Gerhard Heide[1], and Edwin Kroke[2] — [1]TU Bergakademie Freiberg, Institut für Mineralogie, Brennhausgasse 14, 09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Anorganische Chemie, Leipziger Strasse 29, 09599 Freiberg

The new subterranean Shock-Wave-Laboratory at the TU Bergakademie Freiberg (established 2007, extended 2011) opens new vistas for the material synthesis and the investigation of material properties under dynamic loading. Dynamic pressures of >1 Mbar (100 GPa) are a matter of routine. Loading of the samples along the Hugoniot-EOS are as much possibble as the so called "quasistatic loading" or the "reflection method". This opens enhanced possibilities for the material research under extreme conditions. Because this laboratory is localised in the Research- and Teaching Mine "Reiche Zeche", a part of the university, the German mining law for this laboratory is valid. This law together with the status of the university as a research facility ensures contemporary experiments and fast changes of the charge geometries. Cylindrical charges, advanced plane wave generators and hollow explosive charges are possible. Currently this laboratory has experiences in the shock wave synthesis of nano scaled nitrides, shock loading of metals and alloys and the investigation of the results.

MM 4.5 Mon 11:15 H 0106

Severe deformation twinning in pure copper by cryogenic wire drawing — •Alexander Kauffmann[1,2], Jens Freudenberger[1,3], David Geissler[1,2], Song Yin[1,2], Wolfram Schillinger[4], V. Subramanya Sarma[5], Mohsen S. Khoshkhoo[1], Horst Wendrock[1], 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]TU Bergakademie Freiberg, Institute of Materials Science, 09596 Freiberg, Germany — [4]Wieland-Werke AG, Graf-Arco-Straße 36, 89079 Ulm, Germany — [5]Dept. Metallurgical and Materials Engineering, IIT Madras, Chennai 600036, India

The effect of deformation at 77 K on the activation of deformation twinning in pure copper during wire drawing was investigated. For this purpose, cryogenic wire drawing was performed utilizing molyb-

denum disulfide lubrication. Microstructural investigation and texture analysis reveal severe twin formation with broad twin size distribution.

This result is discussed by means of the orientation dependence of deformation twinning in fcc metals and the applied state of stress during wire drawing. Remarkable differences compared to cryogenic rolling with its limited contribution of twinning to grain refinement are highlighted.

MM 5: Transport and Diffusion I

Time: Monday 10:15–11:30 Location: H 1029

MM 5.1 Mon 10:15 H 1029

Investigation of Fe diffusion in Cu by Energy Dispersive X-ray Analysis — •Daria Prokoshkina[1,2], Alexey Rodin[2], and Vladimir Esin[2,3] — [1]Institute for Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Deutschland — [2]Department of Physical-Chemistry, National University of Science and Technology "MISiS", Moscow, Russia — [3]"Département Science et Ingénierie des Matériaux et Métallurgie", Institut Jean Lamour - UMR 7198 - CNRS - Nancy-Université - UPV-Metz, Nancy, France

Iron diffusion in copper is of particular interest since anomalies of iron grain boundary (GB) diffusion in copper have been observed recently. Bernardini et al. [1] investigated Fe GB diffusion in Cu at 716 K after annealing during 96 hours in the B-regime, whereas in the work of Ribbe et al. [2] diffusion annealing at 719 K during 20 hours corresponded to the C-regime. Moreover, a strong curvature of the concentration profiles in Fisher's coordinates was observed by both research groups. In the described works the radiotracer technique was applied. The reasons of the observed anomalies remain unknown. To clarify the problem, another method is used in this work: Energy Dispersive X-ray analysis. GB diffusion measurements are performed in the temperature range from 823 to 1073 K. The parameters of the bulk diffusion of Fe in Cu in the temperature range from 923 to 1273 K are also evaluated. The complex approach of investigating Fe GB diffusion in Cu did not permit to observe fast GB diffusion in the temperature range from 823 to 1073 K. [1] J. Bernardini et al. Def. and Diff. Forum. 249(2006)161. [2] Jens Ribbe et al. Def. and Diff. Forum. 289-292(2009)211.

MM 5.2 Mon 10:30 H 1029

Temperature induced transitions of the grain boundary structure studied by radiotracer diffusion — •Sergiy Divinski[1], Henning Edelhoff[1], Sergey Prokofjev[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Russia

Grain boundary diffusion of ^{110m}Ag in Cu near Σ5 bicrystals is measured parallel and perpendicular to the (001) misorientation axis in both, C and B kinetic regimes after common Harrison's classification. For the first time, the grain boundary diffusion coefficients of a single grain boundary in a true dilute limit of the solute concentration are determined in the C kinetic regime and the values of triple products $P = s \cdot \delta \cdot D_{\mathrm{gb}}$ are measured in the B regime (here s and δ are the segregation factor and the diffusional grain boundary width, respectively). A significant anisotropy of the grain boundary diffusion is established which disappears at the temperatures above 823 K. This temperature corresponds also to a kink in the Arrhenius temperature dependence of the triple product. The phenomenon is discussed in term of a special-to-general transition of the grain boundary structure. The anisotropy of the product $s \cdot \delta$ for a single grain boundary is determined. The effect of non-linear segregation on Ag diffusion in the Cu bicrystal is elucidated via controlled variation of the total amount of the applied tracer material.

The financial support by DFG is acknowledged.

MM 5.3 Mon 10:45 H 1029

Studies of atomic diffusion in crystalline alloys by XPCS — •Markus Stana[1], Michael Leitner[1,2], Manuel Ross[1], and Bogdan Sepiol[1] — [1]Department of Physics, University of Vienna, 1090 Vienna, Austria — [2]Physics-Department E13, TU Munich, 85747 Garching, Germany

X-ray photon correlation spectroscopy is a new method for investigating diffusion on the atomic scale. After our successful application in a Cu-Au single crystal [1], we investigated a Ni-Pt solid solution. As the question of the diffusion mechanism in this system seems settled, the experiment gives good insight in the feasibility and sensitivity of the method. Two samples, a polycrystalline and a single crystal, where prepared and measured at the European Synchrotron Radiation Facility in Grenoble. Activation energy, diffusion coefficient and basic information about the impurity-vacancy interaction has been derived. The talk will give an introduction to XPCS, an overview of our findings and an outlook towards future applications.

[1] M. Leitner, B. Sepiol, L. M. Stadler, B. Pfau, and G. Vogl, Atomic diffusion studied with coherent X-rays, Nature Mat. 8, 717 (2009).

MM 5.4 Mon 11:00 H 1029

Quantitative measurement of the surface diffusion on metallic nanoparticles by aberration-corrected HRTEM — •Alexander Surrey, Darius Pohl, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

Aberration-corrected high-resolution transmission electron microscopy (HRTEM) allows for the investigation of the atomic diffusion on the surface of a nanoparticle in particular during the coalescence of adjacent particles. The incident electron beam may effectively promote this sintering process, although so far, it is not yet known to which extend. Since the material transport during the inter-particle coalescence occurs via surface diffusion, a quantitative determination of the latter is needed. Thus in the present study, the motion of atoms at the surfaces of Au nanoparticles is characterized by means of aberration-corrected HRTEM with the resolution of individual atomic columns. Subjects of the analysis are Au icosahedra on amorphous carbon substrates and single crystalline Au octahedra whose surfaces extend into the vacuum and which are thus imaged "without a substrate". A method is developed which allows for a quantitative estimation of the diffusion coefficient based on the measured temporal fluctuation of the occupation of individual atomic surface columns as obtained from HRTEM images. The likewise derived coefficient of the surface self-diffusion is in very good agreement with the results of atomic force and scanning tunneling microscopy studies.

MM 5.5 Mon 11:15 H 1029

Diffusion of charged point defects upon long-range coulomb interaction made simple — •Hannes Guhl, Paul Tangney, W.M.C. Foulkes, and Michael W. Finnis — Department of Physics and Materials, Imperial College London, London

Migration of charged point defects has been a long standing issue as it controls mass transport and ionic conductivity in insulators in various technological applications, such as gas sensors and solid oxide fuel cells. However, many stochastic studies aiming to model defect kinetics based on atomistic or first-principles information treat the mutual coulomb interaction only very roughly or neglect it altogether, as the long-range character is awkward to handle within the usually applied lattice models. Therefore, we have developed, on the basis of Debye-Hückel-theory, an intuitive and easy-to-use method to describe the diffusion of fully interacting charged point defects in an otherwise perfect crystal. As an example we apply this to a model oxide material doped with aliovalent foreign atoms. Within a systematic error smaller than one order of magnitude, the proposed formula correctly describes the data obtained from extensive Kinetic Monte Carlo simulations over a wide range of defect concentrations and temperatures. Furthermore, we demonstrate that the long-range character of the coulomb interaction gives rise to a lower bound of the diffusivity as the dopant concentration increases at constant temperature. This suggests that conventional techniques treating the defect-defect-interactions may significantly underestimate the mobility of charged species in ionic materials.

MM 6: Mechanical Properties II

Time: Monday 11:30–12:45 Location: H 0106

MM 6.1 Mon 11:30 H 0106

Dislocation microstructure evolution and size effect during torsion of thin single crystalline metallic wires: a discrete dislocation dynamics approach — Jochen Senger and •Daniel Weygand — Karlsruhe Institute of Technology, IAM, Karlsruhe, Germany

The ground breaking investigations of Fleck [1] on the size dependence observed by applying torsion boundary constraints have – to the authors knowledge – not been addresses by 3D discrete dislocation dynamics (3DDD). Under torsion, the trend smaller is stronger has been found. This observation has been a motivation for strain gradients approaches. Despite this a detailed knowledge on the dislocation microstructure, characteristic for torsion is lacking. Therefore we report on the hardening with twist angle and on dislocation microstructures under twist loading and unloading for single crystals obtained by 3DDD [2].

[1] N. A. Fleck, G. M. Muller, M. F. Ashby, and J. W. Hutchinson. Acta Met. 42 (1994) 475.

[2] J. Senger, D. Weygand, O. Kraft, P. Gumbsch, *Dislocation microstructure evolution in cyclically twisted microsamples: a discrete dislocation dynamics simulation*, Modelling Simul. Mater. Sci. Eng. 19 (2011) 074004.

MM 6.2 Mon 11:45 H 0106

Existence of Two Twinning-Mediated Plastic Deformation Modes in Au Nanowhiskers — •Erik Bitzek[1], Andreas Sedlmayr[2], Daniel S. Gianola[3], Gunther Richter[4], Reiner Mönig[2], and Oliver Kraft[2] — [1]WW1, Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg — [2]Institute for Applied Materials, Karlsruhe Institute of Technology — [3]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA — [4]Max-Planck-Institut for Intelligent Systems, Stuttgart

Single crystalline metallic nanowhiskers have lately attracted substantial interest due to their special mechanical properties. Here we report on in situ tensile experiments and molecular dynamics (MD) simulations on nominally defect-free single-crystalline Au nanowhiskers in [110] orientation. The room temperature experiments reveal strengths on the order of the ideal strength and plastic strains of up to 12%; a direct result of deformation twinning that is shown to govern the plastic flow. This is in clear contrast to the situation in coarse-grained fcc metals, where twinning is only observed at very low temperatures or at very high strain rates. The in situ and post mortem electron microscopy observations furthermore show two broad classes of deformation morphologies that correlate with distinct stress-strain responses. MD simulations show that the mechanism of twin growth can change from layer-by-layer propagation to parallel and accelerated formation of coalescing nanotwins.

MM 6.3 Mon 12:00 H 0106

Nano mechanical surface properties of the ferromagnetic shape memory alloy Ni-Mn-Ga — •Alexander Malwin Jakob and S.G. Mayr — Leibniz-Institut für Oberflächenmodifizierung, Translationszentrum für regenerative Medizin und Fakultät fuer Physik und Geowissenschaften der Universität Leipzig, 04318 Leipzig

During the last two decades, the wide field of so called "smart materials" attracted more and more interest in solid state physics. Ni-Mn-Ga, a ferromagnetic shape memory alloy (FMSM) - well known for its strong magneto-elastic coupling - yields high reversible strains up to 10% at external magnetic fields around 1 T [1]. Despite intensive investigations, nano scale processes causing magnetic shape memory effect still call for more detailed observation. Epitaxial grown 14M Ni-Mn-Ga thin films by magnetron sputtering are scope of our work. We investigate local indentation module M by means of contact resonance atomic force microscopy (CR-AFM) [2,3]. Experimental data are compared to theoretical predictions based on density functional theory (DFT). A discussion in context of super elasticity and phase transformations is given. This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909

[1] Sozinov A., Likhachev A.A., Lanska N., and Ullakko K., Appl. Phys. Lett. Vol. 80, no. 10 (2002)

[2] Rabe U., Arnold W., Appl. Phys. Lett. Vol.64, P1493-1495 (1994)

[3] Yamanaka K., Ogiso H., Kolosov O., Appl. Phys. Lett., Vol.64, P178-180 (1994)

MM 6.4 Mon 12:15 H 0106

ab initio study of the mechanical shear behavior of Al with and without normal stresses — •Xueyong Pang, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Bochum, Germany

To investigate the mechanical shear properties of interfaces in metals we have determined the gamma-surfaces of different special tilt and twist grain boundaries in aluminum by means of ab-initio calculations. From the gamma-surfaces we obtained minimum energy paths and barriers, as well as the theoretical shear strength. For the [110] tilt grain boundaries, the theoretical shear strength scales with the height of the slip barrier and exhibits a relation with the misorientation angle: the closer the angle to 90°, the higher the shear stress. To estimate the effect of full atomic relaxation, we carried calculations of the theoretical shear strength of Al single crystals in the (111) plane by different deformation methods. To investigate the influence of normal stresses on the shear behavior of Al, we also performed a series of combined normal/shear calculations on single crystal Al and grain boundaries. The critical shear strength follows the linear relationship with the normal stress; the critical shear strength decreases with the compression stress decreases and the tensile stress increases.

MM 6.5 Mon 12:30 H 0106

Ultrasensitive detection of biomolecules using Al nanostructures as SERS substrates — •Shankar Kumar Jha[1], Yasin Ekinci[1,2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

Surface-enhanced Raman scattering (SERS) is an important technique for detecting molecules at low concentrations. The commonly used excitation sources are visible and near-infrared lasers since the frequently used SERS substrates support strong localized surface plasmon resonances (LSPR) at these wavelengths. Most of the biologically important molecules exhibit strong absorption in the deep-ultraviolet (DUV) wavelength region, giving rise to resonance Raman effect. Thus, apart from the increased Raman cross-sections and elimination of the prevalent fluorescence background, the use of DUV excitation would offer the possibility of combining the advantages of resonance Raman and SERS effects leading to surface-enhanced resonance Raman scattering (SERRS). We explore the use of designed aluminum nanoparticles as SERS substrates in the DUV region. The nanoparticle arrays fabricated over large areas using extreme-ultraviolet interference-lithography (EUV-IL) exhibit sharp and tunable LSPR in the UV and DUV wavelength ranges and allows for reproducible enhancement of Raman signal from molecules coated on these arrays. We demonstrate ultrasensitive and real-time analytical detection of biomolecules using these designed Al nanostructures as SERS substrates.

MM 7: Transport and Diffusion II

Time: Monday 11:30–12:45 Location: H 1029

MM 7.1 Mon 11:30 H 1029

First-principle study and modeling of strain dependent ionic migration on ZrO_2 — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Electrolytes with high ionic conductivity at lower temperatures are the prerequisite for the success of Solid Oxide Fuel Cells (SOFC). One promising candidate is doped zirconia. In the past its ionic conductivity has mainly been increased by decreasing its thickness. However, the influence of the thickness is only linear whereas the impact of migration barriers is exponential. Therefore understanding the oxygen transport in doped zirconia is of fundamental importance. In this work we pursue the approach of the strain dependent ionic migration in zirconia. We investigate how the migration barriers for oxygen ions respond to a change of the atomic strain. We employ the method of Density Functional Theory (DFT) to obtain the migration barrier of the oxygen ion jumps in zirconia for a given lattice constant. In contrast to other publications we find a migration barrier decrease for high compressive strains beyond a maximal height of the migration barrier at an intermediate compressive strain. We present a simple analytic model which by using interactions of the Lennard Jones type gives an explanation for this behavior.

MM 7.2 Mon 11:45 H 1029

The influence of Mg and Si atoms on the cluster formation process in Al-Mg-Si alloys studied by positron annihilation lifetime spectroscopy — •Meng Liu[1,2], Yong Yan[2], Zeqin Liang[1], Cynthia Chang[2], and John Banhart[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin — [2]Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

After natural ageing (NA), Al-Mg-Si alloys with various Mg and Si contents exhibit either positive or negative strength response during subsequent artificial ageing, which is caused by clusters formed during NA. Previous studies focused on cluster formation in Al-Mg-Si alloys by using Positron Annihilation Lifetime Spectroscopy (which is uniquely sensitive to vacancies) found that the entire evolution consists of at least 4 stages. However, the exact interpretation of the underlying microscopic processes is still under dispute. Therefore, in-situ positron lifetime experiments were carried out for pure Al-Mg and Al-Si binary alloys with solute concentrations ranging from 0.005 at.% to 1 at.% in order to clarify the behaviour of Mg/Si atoms on the clustering formation processes from a vacancy perspective. The results show that in general, a decrease in positron lifetime to a stable value after a certain period of NA for both alloying systems can be observed. Lifetimes of Al-Mg samples are significantly higher than in Al-Si alloys for equal solute content. In addition, these results are compared to the Differential Scanning Calorimetry results for getting a better understanding of the different clustering stages in Al-Mg-Si alloys.

MM 7.3 Mon 12:00 H 1029

Simulation of internal nitradation phenomena with a cellular automata approach — •Katrin Jahns, Martin Landwehr, Jürgen Wübbelmann, and Ulrich Krupp — University of Applied Sciences Osnabrück, Faculty of Engineering and Computer Science, Albrechtstrasse 30, 49076 Osnabrück, Germany

In this study a simulation program is developed for predicting precipitation accompanying diffusion processes based on the method of cellular automata. Hereby, nitrogen diffusion and precipitate formation are simulated individually and in combination. Operation of high-temperature components as well as surface hardening processes, e.g., carburizing and nitridation, involve diffusion of gases in metals and alloying elements, precipitate nucleation and growth. The higher specific volume of the internal precipitates as compared to the substrate causes the generation of residual compressive stresses in the surface layer. Besides thermodynamics, these effects are taken into account when evolving the program. The simulation program is evaluated and verified by means of thermogravimetric nitridation and carburization experiments.

MM 7.4 Mon 12:15 H 1029

Transport Properties of In_2O_3 and its surface electron accumulation layer — •Natalie Preissler, Oliver Bierwagen, and James. S. Speck — preissler@pdi-berlin.de

We used variable temperature Hall measurements and room temperature thermoelectric measurements to determine the transport properties (mobility, sheet resistance, charge density, Seebeck-coefficient) of In_2O_3 thin films and their surface electron accumulation layers (SEALs). SEALs have an important impact on device applications and were shown already by x-ray photoelectron spectroscopy (XPS) and current-voltage (I-V) measurements, while their actual transport properties are still unknown. The investigated In_2O_3 samples were about 500 nm thick and were grown on insulating Yttria-stabilized zirconia (YSZ) by plasma-assisted molecular beam epitaxy. Unintentionally doped (uid) In_2O_3 exhibits n-type conductivity with a significantly lower volume electron concentration than in the SEAL. Acceptor doping by Mg turned the bulk of the samples insulating to maximize the relative contribution of the SEAL to the total conductivity. As a result we can estimate the sheet resistance of the SEAL to be greater than 46 kΩ. Current-voltage measurements with Hg contacts showed the existance of the SEAL. Temperature dependent Hall measurements were used to differentiate between the degenerate SEAL (high volume electron concentration, no freeze-out) and non-degenerate bulk (low concentration, freeze-out). While Hall measurements give a total sheet electron concentration, the Seebeck coefficient is related to the volume electron concentration and is used as another indicator for the SEAL.

MM 7.5 Mon 12:30 H 1029

Critical current noise in rough Josephson junctions — •Pierre-Luc Dallaire-Demers[1], Mohammad Ansari[2], and Frank Wilhelm-Mauch[1] — [1]Universität des Saarlandes, Saarbrücken, Deutschland — [2]University of Waterloo, Waterloo, Canada

While dissipationless, Josephson junctions as elements in superconducting nanocircuits are plagued by intrinsic noise mechanisms that will limit the coherence time of future high-precision quantum devices. Significant sources of current fluctuations may be caused by the noncristallinity and disorder of the oxide layer separating the two superconducting leads. A microscopic calculation of the spectral density of noise of a rough superconducting tunnel junction is presented in this work. To account for disorder, a Josephson junction is modelled as a set of pinholes with a universal bimodal distribution of transmission eigenvalues that add their noise power incoherently. Each pinhole is treated as a ballistic point contact with an intrinsic thin barrier that modulates the transmission coefficient. The noise spectrum is computed using the quasiclassical Green's function method for non-equilibrium superconductivity. This formalism allows us to investigate high and low transmission limits at finite temperature for any relevant frequency. As suggested by experiments, low transmission pinholes generate shot noise while fast switching between the subgap states of high transmission channels create a strong non-poissonian low-frequency noise yet to be measured. The fluctuation of the low-frequency noise from one sample to the other is also found to be significant when the phase of the order-parameter is anti-symmetric across the junction.

MM 8: Computational Materials Modelling II - Methods

Time: Monday 11:45–13:00 Location: TC 006

MM 8.1 Mon 11:45 TC 006

Discontinuous epitaxial Bain paths and consequences for coherent epitaxial growth — •Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Strained coherent epitaxy is a valuable mean to influence structural, electronic, magnetic and optical properties of bulk-like films as a function of symmetry and in-plane lattice spacings of the substrate. A

remarkable example are 50 nm thick films of body centred tetragonal (BCT) $Fe_{70}Pd_{30}$, whose ferromagnetic properties, e.g. magnetic moment and magnetic anisotropy, can be tuned by the choice of the substrate (Buschbeck *et al.*, PRL **103**, 216101 (2009)). This tuning extends over a wide range of tetragonal distortion in the film, $1.09 \leq c/a \leq 1.54$ (Kaufmann-Weiss *et al.*, PRL **107**, 206105 (2011)).

From the point of theory, an epitaxial Bain path (EBP) models the bulk part (i.e. the interior) of films in BCT structure coherently grown on substrates with four-fold symmetry by establishing a relationship between the substrate lattice parameter, a, and the out-of-plane lattice parameter of the film, c (Alippi *et al.*, PRL **78**, 3892 (1997)). We show in this contribution using several examples of the transition metal family, that c need not be a continuous function of a, hence the c/a ratio in BCT films of these elements cannot continuously be adjusted giving rise to a discontinuous EBP. Calculations of the electronic structure in the framework of density functional theory were carried out in the implementation of the full potential local orbital program package FPLO (www.fplo.de).

MM 8.2 Mon 12:00 TC 006

An evolution strategy for crystal structure prediction — •Silvia Bahmann, Thomas Gruber, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

The crystal structure determines many physical properties. For materials design of new systems with a given chemical composition one therefore needs the ability to predict possible crystal structures. The challenge in this prediction lies in the facts that it is a global search in a search space that grows exponentially with the number of atoms per unit cell and the unknown energy landscape containing several minima.

Our evolutionary strategy uses the main features of natural evolution - recombination, mutation, selection and the survival of the fittest - to global search. The crystal structures represent the individuals in this picture whereas their fitness value is determined by calculating the free energy of the individual using electronic structure programs. The individual having the minimal free energy in the whole search space is considered to be the most stable structure. The combination of the effective local optimisation already implemented in electronic structure programs with stochastic elements of the evolution strategy ensures an efficient search.

We present the developed evolution strategy designed for general 3D crystal structure prediction that also features the search of 2-dimensional structures. As an application we focus here on the search for 3D structures of lithium-silicides that are promising for new electrode materials for lithium ion batteries.

MM 8.3 Mon 12:15 TC 006

Fingerprinting defects and structures in atomistic simulations — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Employing atomistic simulations to investigate structural phase transformations in solids is a challenging task. A prerequisite for analysing the simulation results is the ability to locally identify structures and structural features. It is then possible to find point and extended defects and to track e.g. the movement of an interface between two structures during a phase transformation. To address this problem we have implemented a polyhedron analysis method. Within our approach we analyse the local coordination polyhedra around each atom and establish a fingerprint that reflects the arrangements of polyhedra within the polyhedron network. The distribution of polyhedra in a structure together with the fingerprint then provides sufficient information to classify a given structure.

The polyhedron analysis method is based on the distinct geometrical features of complex phases that form in metal alloys. The formation and growth of such complex phases is of particular interest since they can significantly influence the materials properties. Insight on the atomistic level provides valuable information on the underlying microscopic processes. We have applied our polyhedron analysis in molecular dynamics and adaptive kinetic Monte Carlo simulations, to track vacancies, monitor phase growth, identify interfaces and follow their motion.

MM 8.4 Mon 12:30 TC 006

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 including magnetism has yet to be developed for the Fe-C interaction. Although interatomic potentials have been obtained for this system, 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 then down-folded onto an 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 interstitial carbon in Fe-structures can be achieved. Furthermore, we use the model to calculate elastic properties and energies of a variety of Fe-carbides, defects, and carbon diffusion paths. This simple model based on physical insights may be used to study systems containing thousands of atoms.

MM 8.5 Mon 12:45 TC 006

A novel minimum search method for complex optimization problems — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Optimization is essential in many scientific and economical areas, as well as in the development of products. In many cases the optimization problem is too complex to be tackled by simple straight forward calculations or by trial and error. The reason is the too large phase space of the optimization problem and a rough potential surface with too many local minima. To find the global minimum, or at least a representative one, there are methods like simulated annealing, which has the chance to escape local minima, or the genetic algorithm, which changes the configurations by combining subsets of different deep minima. The chance to get stuck in a local minimum or to escape is proportional to the depth of the minimum in these methods.

Here we present a new method, which is complementary to the established ones. The chance to get stuck in a local minimum or to escape is independent of the minimum's depth but depends on the minimum's attractor size. Therefore, it can overcome local minima and high barriers equally well. Even though it does not get stuck in local minima of small attractor size, it is especially advantageous when searching for a minimum with a small basin of attraction. We successfully applied the method to find the ground states of the phosphorus P_4 and P_8 molecules as well as the arsenic As_4 and As_8 molecules. In the case of P_8 we were able to find a new stable configuration.

MM 9: Topical Session Bulk Nanostrucured Materials II - Processing

Time: Monday 11:45–13:00 Location: H 0107

Topical Talk MM 9.1 Mon 11:45 H 0107

Tailoring and grading materials properties by Accumulative Roll Bonding — •Heinz Werner Höppel and Mathias Göken — Dept. of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, 91058 Erlangen, Germany

Accumulative roll bonding (ARB) is a very promising and also prominent process to produce ultrafine-grained sheet materials in larger quantities. During the last decade, strong progress was made in processing technology combined with a much deeper understanding of the microstructural evolution during ARB-processing. Besides this well-known conventional route of ARB-processing, new concepts have been derived to produce multiphase, tailored or graded sheet materials with promising properties. By an intelligent ARB-processing 3D-architectured multiphase materials can be achieved aiming for locally tailored materials properties. It is shown, that the materials properties can be tailored locally by an adopted powder spraying process via the ARB process. Moreover, by using an appropiate post ARB-heat treatment, this technique can aslo be used to strengthen the sheet material by the formation of intermatallic phases in the sheet. In the talk, mi-

crostructural and mechanical properties with respect to the processing parameters will be discussed in detail.

MM 9.2 Mon 12:15 H 0107

Severe plastic deformation of NiAl by high pressure torsion — •David Geist, Christoph Gammer, Hans-Peter Karnthaler, and Christian Rentenberger — Universitys of Vienna, Physics of Nanostructured Materials, Boltzmanng. 5, 1090 Wien, Austria

Severe plastic deformation is an important process to render bulk materials nanostructured. In this work, the B2-ordered intermetallic compound NiAl is subjected to a high pressure torsion deformation at room temperature. The structure of NiAl after different amounts of shear deformation is studied using light microscopy, scanning and transmission electron microscopy. Plan view and cross-section samples are investigated for a local analysis of the occurring micro- and nanostructures. It is shown that high pressure torsion deformation of NiAl leads to different fragmented structures that are inhomogeneously distributed in the cross-section samples. In some regions, ultra-fine grained and nanocrystalline structures are observed. Contrary to B2 ordered FeAl [1], no indications of deformation-induced disordering were encountered. This difference in disordering behaviour is attributed to the dissociation modes of the glide dislocations with and without antiphase boundaries in FeAl and NiAl, respectively. It is shown that high pressure torsion can be used to severely refine the structure even in the case of a brittle compound like NiAl.

[1] C. Gammer et al. (2011) Scripta Materialia 65 (1) 57. The authors thank Dr. Sergiy Divinski, Institute for Materials Physics, University of Munster, for the kind provision of NiAl samples and acknowledge support by the Austrian Science Fund (FWF):[P22440, S10403]

MM 9.3 Mon 12:30 H 0107

Solid state amorphization of bulk Co_3Ti using high pressure torsion — Christoph Gammer, David Geist, Christian Rentenberger, and •Hans-Peter Karnthaler — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Amorphous structures can be achieved by a solid state transformation of the crystalline structure using severe plastic deformation. This has been proven to be successful by applying high pressure torsion (HPT) deformation in the case of $L1_2$ ordered Zr_3Al [1]. In addition, a cyclic transformation from crystalline to amorphous and back to a crystalline phase was reported to occur in Co_3Ti upon high-energy ball milling of a mixture of elemental powders [2]. In the present study bulk material of intermetallic Co_3Ti is transformed locally to an amorphous phase by HPT deformation. The deformation structures are analysed on different length scales using both scanning and transmission electron microscopy (TEM) methods. To avoid crystallization during preparation, the TEM samples were prepared electrochemically. They show amorphous bands that contain a debris structure of small grains ($\sim$ 5 nm) as in Zr_3Al. In addition, the presence of some large ($\sim$ 50 nm) defect free grains occurring in the amorphous bands indicate the reverse transition from an amorphous phase back to a crystalline one.

[1] D. Geist, C. Rentenberger, H. P. Karnthaler. Acta Mater. 59, 4578 (2011) [2] M. Sherif El-Eskandarany, K. Aoki, K. Sumiyama, K. Suzuki. Acta Mater. 50, 1113 (2002). This work was supported by the Austrian Science Fund (FWF): [P22440].

MM 9.4 Mon 12:45 H 0107

SPD processed ß-TiNb alloys for biomedical applications — •Ajit Panigrahi[1], Thomas Waitz[1], Erhard Schafler[1], Matthias Bönisch[2], Mariana Calin[2], Annett Gebert[2], Jürgen Eckert[2,3], Werner Skrotzki[4], and Michael Zehetbauer[1] — [1]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Austria — [2]Institut für Komplexe Materialien, IFW Dresden, Germany — [3]Institut für Werkstoffwissenschaft, TU Dresden, Germany — [4]Institut für Strukturphysik, TU Dresden, Germany

The scientific goals of the recently established EU MC training network "BioTiNet" comprise the development of nanocrystalline and amorphous ß-Ti alloys for medical implants. Using methods of severe plastic deformation, it is the aim to process novel materials that show a tailored combination of high strength, considerable ductility, biocompatibility and low Young's modulus. A low value of Young's modulus of the ß-Ti-Nb alloys close to that of bone is a prerequisite for applications as materials for prosthesis minimizing stress shielding effects. ß-Ti-Nb based alloys including "gum metals" are of special interest. These materials also offer the possibility to accommodate elastic strains via superelasticity occurring by a martensitic phase transformation. This work reports on first results obtained by mechanical investigations of ß-Ti-Nb alloys of selected compositions which have been processed by HPT and ARB. X-ray profile analyses using synchrotron radiation is used to analyse the mechanisms of plastic deformation where dislocations seem to play only a minor role. Work supported within the EU Programme FP7/2007-13 under grant agreement No. 264635 (BioTiNet-ITN)

MM 10: HV Wagner

Time: Monday 15:00–15:30 Location: H 0107

Invited Talk MM 10.1 Mon 15:00 H 0107

Microstructural and mechanical anisotropy of ultra fine grained metals and alloys after ECAP — •Martin Wagner and Matthias Hockauf — Institut für Werkstoffwissenschaft und Werkstofftechnik, TU Chemnitz, Deutschland

Severe plastic deformation of metals and alloys by equal-channel angular pressing (ECAP) produces ultra fine grained (UFG) microstructures that often exhibit excellent mechanical properties. However, various subtle requirements make the processing technique challenging both from a materials engineering and a materials science point of view. While research on UFG materials has been en vogue for quite some time, many fundamental aspects relating microstructural evolution and macroscopic behavior are not fully understood today. In this contribution, we present recent results that provide novel insights into the ECAP technique and the mechanical behavior of UFG materials: (i) we study the effect of back-pressure during ECAP on microstructural homogeneity and anisotropy of Cu and Al-alloys; (ii) we document the evolution of texture, grain size and mechanical properties in a Mg alloy; (iii) we discuss how up-scaling of the ECAP technique to technologically relevant specimen sizes results in gradients and microstructural heterogeneity in large billets; (iv) we use the large-scale ECAP technique to deform specimens along novel, truly 3 dimensional strain paths that activate a larger number of shear planes than the common ECAP paths.

MM 11: Joint Session FePt Nanoparticles (jointly with DS, MM)

Time: Monday 15:00–17:45 Location: EB 202

Topical Talk MM 11.1 Mon 15:00 EB 202

Prediction of morphology-, composition- and size-related trends in FePt nanoparticles from first principles — •Markus Ernst Gruner — Faculty of Physics and Center for Nanointegration CeNiDE, University of Duisburg-Essen, 47048 Duisburg

Owed to the large magneto-crystalline anisotropy (MCA) of bulk FePt alloys, nanostructures with effective diameters as small as 4 nm are considered for ultra-high density recording applications. Structural defects as multiple twinning, segregation and partial ordering effectively reduce the MCA and thus severely limit the integration density. First principles calculations in the framework of density functional theory permit independent insight into the size-dependent interrelation between composition, structural stability and magnetism granting access to the electronic level. Site-resolved orbital moments and MCA are obtained a fully relativistic treatment including spin-orbit interaction.

Large scale calculations with up to 1415 atoms demonstrate that for

diameters around 4 nm a close competition between multiply twinned and single crystalline morphologies is present, while the low energy of Pt surfaces enhances segregation. The systematic variation of 3*d* and 5*d* components reveals that especially addition of Mn can reduce twinning, while complicating the magnetic configuration. Structural and electronic changes which may degrade the magnetic properties must also be expected from a protective encapsulation with main group elements.

Topical Talk MM 11.2 Mon 15:30 EB 202
Coulomb Blockade effects in FePt nanoparticles — •Artur Erbe[1], Ulrich Wiesenhütter[1], Darius Pohl[2], Bernd Rellinghaus[2], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]IFW Dresden

In order to correlate the size and crystallinity of FePt nanoparticles with their respective electrical and mangeto-electrical properties individual nanoparticles are contacted using electron beam lithography. The particles are prepared from gas phase on electron transparent SiN membranes which allows the transmission electron microscopy of the same nanoparticle which is characterized electrically. The fabrication results in junctions, in which single FePt nanoparticles are connected to external leads. These junctions are tested electronically by measuring the current-voltage characteristics at various gate voltages, temperatures and magnetic fields. We observe Coulomb Blockade effects which are in agreement with the dimensions obtained from the TEM studies. The results of the magnetic nanoparticles are compared to measurements taken on Au nanoparticles of similar sizes.

Topical Talk MM 11.3 Mon 16:00 EB 202
Pt surface segregation and its impact on magnetism in FePt nanoparticles — •Ulf Wiedwald — Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The appealing magnetic properties of chemically ordered FePt alloys strongly depend on composition. In nanoparticles with diameters below 10 nm the relative number of surface-near atoms strongly increases, thus any tendency of segregation will significantly change the stoichiometry of the interior. As a result, magnetic moments as well as magnetic anisotropy may vary compared to the bulk. In the frame of the collaborative research center SFB 569 we prepared size-selected, hexagonally arranged metallic particles by precursor loaded reverse micelles and plasma etching [1]. Pt segregation [2] and its impact on magnetism were examined in-situ for naked, non-interacting FePt particles on Si/SiO_2 as function of size (2-10nm) by photoelectron spectroscopy and x-ray magnetic circular dichroism. For partially $L1_0$-ordered particles we observe reduced spin moments with decreasing diameter while the orbital moment is found rather independent of size. As connected to the orbital magnetism, the effective magnetic anisotropy is also conserved for decreasing diameters, though reduced relative to the bulk [3]. Reasons for these astonishing observations are discussed.
[1] A. Ethirajan, U. Wiedwald, et al., Adv. Mater. 19, 406 (2007).
[2] L. Han, U. Wiedwald, B. Kuerbanjiang, P. Ziemann, Nanotechnology 20, 285706 (2009).
[3] U. Wiedwald, L. Han, J. Biskupek, U. Kaiser, P. Ziemann, Beilstein J. Nanotechnol. 1, 24 (2010).

Topical Talk MM 11.4 Mon 16:30 EB 202
Understanding the Metal-Carbon Interface in FePt terminated carbon nanotubes — •Darius Pohl[1], Franziska Schäffel[1], Christine Täschner[1], Marc H. Rümmeli[1], Christian Kisielowski[2], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, P.O. Box 270116, Dresden, D-01171, Germany — [2]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Plasma-enhanced chemical vapour deposition (PE-CVD) onto FePt catalyst films is used to synthesize carbon nanotubes (CNT) which are teminated with L10-ordered FePt nanomagnets with high magnetic anisotropy [1]. The CNT are characterized by means of low voltage aberration-corrected HRTEM. To gain a deeper insight into the growth mechanism and in order to understand the relative crystallographic orientation of the particles with respect to the CNT axes structural investigations are conducted with a strong focus on the atomically resolved characterisation of the FePt-CNT interface. An interface-near expansion of the metal lattice is observed and attributed to a segregation of Pt towards the surface of the catalyst particle. Detailed statistical HRTEM analyses of these interfaces reveal that the CNT preferentially emanate from {111} facets of the catalyst particle. Molecular dynamic simulations were conducted to estimate the desorption energy of carbon atoms for various surfaces. Our results indicate that the physical principle based upon which the interfacial metal facet is chosen is a reduction of the desorption energy for carbon [2].
[1] F. Schäffel et al., Appl. Phys. Lett. 94 (2009) 193197.
[2] D. Pohl et al., Phys. Rev. Lett. 107 (2011) 185501.

Topical Talk MM 11.5 Mon 17:00 EB 202
Atomistic characterisation of ultrahard nanomagnets — •Carolin Antoniak — Experimentalphysik/AG Wende and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

A combination of x-ray absorption spectroscopy (XAS) and density functional theory (DFT) has been used to study the magnetic properties like spin and orbital magnetic moments and effective magnetocrystalline anisotropy of chemically ordered FePt nanoparticles on an atomistic lengthscale. By choosing the appropriate capping material, these properties can be tuned between hard and soft magnetic with either high or low magnetic moments [1]. Focus of this talk will be the results of XAS allowing for an element-specific analysis of magnetic properties. Complemented with DFT calculations, it helps to gain more insight to the mutual influence of nanoparticles and capping material allowing to state design guidelines for improved materials which will be presented in this contribution.

This work was done in collaboration with M.E. Gruner, M. Spasova, A. Rogalev, F. Wilhelm, A.V. Trunova, F.M. Römer, A. Warland, B. Krumme, K. Fauth, S. Sun, P. Entel, M. Farle, and H. Wende. We thank the HZB-BESSYII and ESRF staff as well as the staff of the Jülich Supercomputing Center, and P. Vezolle of IBM for their kind support. Funded by BMBF (05 ES3XBA/5), EU and DFG (SFB445, SPP1239)

[1] C. Antoniak, M.E. Gruner et al., Nature Comm. 2, 528 (2011)

15 min. break

MM 12: Joint Symposium 100 years of X-ray diffraction: from the Laue experiment to new frontiers (jointly with KR, BP, CPP, DF, MA, MM, GP)

Time: Monday 15:00–17:30 Location: H 0105

Invited Talk MM 12.1 Mon 15:00 H 0105
Disputed discovery: The beginnings of X-ray diffraction in crystals — •Michael Eckert — Deutsches Museum, Forschungsinstitut, Museumsinsel 1, D-80538 München

The discovery of X-ray diffraction in crystals was based on misconceptions about the nature of X-rays. The background of "Laue's discovery" and its early repercussions are described from the perspective of contemporary views in 1912. The riddle concerned the origin of the monochromacy observed in the Laue spots.

Invited Talk MM 12.2 Mon 15:30 H 0105
Why are quasicrystals quasiperiodic? — •Walter Steurer — Laboratorium für Kristallographie, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Schweiz

It took more than two years until Dan Shechtman could publish his finding of a rapidly solidified Al-Mn phase with sharp Bragg reflections and icosahedral point group symmetry. His results were not accepted, initially, since they seemed to contradict fundamental laws of crystallography. A further twenty-seven years had to pass by until his discovery of quasicrystals was honoured by the Nobel Prize in 2011. This discovery was fundamental because quasiperiodic order represents a novel equilibrium state of solid matter fundamentally different from the common periodic one.

At present, stable quasicrystals have been found in more than fifty binary and ternary intermetallic systems. They show mostly decagonal or icosahedral diffraction symmetry contrary to soft quasicrystals. These are mainly qasiperiodic structures resulting from the self-assembly of either micelles in a liquid or of terpolymers with dodecago-

nal symmetry. The so far most promising applications of quasiperiodic structures seem to be in the field of photonic and phononic crystals.

The focus of the talk will be on the driving forces for the formation and stablization of quasiperiodic structures.

Invited Talk MM 12.3 Mon 16:00 H 0105

Coherent Diffraction Imaging with Free-Eletron Lasers — •Massimo Altarelli — European XFEL GmbH, 22607 Hamburg

One hundred years after the discovery of x-ray diffraction from crystals, spatially coherent, ultra-brilliant and ultra-short pulses of x-ray radiation from free electron lasers (FEL's) open the way to structure solution without the hurdle of crystallization. Biological objects such as cells, viruses, possibly down to individual macromolecules and to atomic resolution, and individual nanostructures in material sciences are eligible for these novel studies. An overview of the x-ray FEL sources and their basic physical principles and properties, of the strategies for sample handling and data collection and a glimpse of the necessary algorithms to phase the diffraction patterns are given. Example of results from the soft x-ray FLASH source in Hamburg and from the Linac Coherent Light Source in Stanford are illustrated. The perspectives and the challenges of the high repetition rate (up to 27 000 pulses/s) of the European XFEL, under construction in the Hamburg region, are also briefly discussed

Invited Talk MM 12.4 Mon 16:30 H 0105

X-ray free-electron lasers - emerging opportunities for structural biology — •Ilme Schlichting — Max Planck Institute for Medical Research, Heidelberg, Germany

X-ray crystallography is a mature yet still advancing method for structure determination of molecules with any molecular weight. Facilitated greatly by synchrotron X-ray sources, the method is limited only by the quality and size of the crystals and by radiation damage. Free-electron lasers (FELs) provide orders of magnitude brighter and shorter X-ray pulses than conventional synchrotron sources. It has been proposed that radiation damage, which limits the high resolution imaging of soft condensed matter, can be "outrun' by using ultrafast and extremely intense X-ray pulses that pass the sample before the onset of significant radiation damage [1]. Thus, one of the most promising scientific applications of XFELs is in sub-nanometer resolution imaging of biological objects, including viruses, macromolecular assemblies, and nanocrystals. The concept of "diffraction-before-destruction" has been demonstrated recently at the Linac Coherent Light Source (LCLS) [2], the first operational hard X-ray FEL, for protein micro- and nanocrystals [3] and single mimivirus particles [4]. These experiments and recent developments and progress will be presented.

[1]. Neutze et al., Nature 406, 752-757 (2000). [2]. Emma, Nature Photonics 4, 641-647 (2010). [3]. Chapman et al., Nature 470, 73-77 (2011). [4]. Seibert et al., Nature 470, 78-81 (2011).

Invited Talk MM 12.5 Mon 17:00 H 0105

Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling — •Tim Salditt — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Classical x-ray diffraction has been based on three constraints: (i) averages over macroscopic accumulation time and sample sizes, which are many orders of magnitude larger than the structures to be resolved; (ii) homeogeneous "well ordered" samples which are - if not crystalline - characterized by well-defined correlation functions; (iii) data analysis by fitting to modeled diffraction data. However, many condensed matter problems, in particular in functional materials, soft matter and biomolecular samples, address non-equilibrium states with competing length scales, hierachical structures, and intrinsic dynamics. Progress in x-ray sources and optics has helped to meet these challenges. Conceptually often still close to the Laue experiment, far-field diffraction data can now be collected in controllable field of vies, with highly focused beams reaching the 10 nm range. Biomolecular diffraction signals can be recorded from hierachical structures such as a biological cells. Perhaps most importantly, fully coherent illumination enables data inversion without prohibitive model building. How these advances serve science, will be illustrated by examples in neuro-biophysics. We present experiments addressing different structural levels and bridging length scales, from proteins and lipid assemblies up to a complete organelle such as the synaptic vesicle, from an isolated axon up to an unsliced nerve, from tissue slice to the sensory organ.

MM 13: Computational Materials Modelling III - Alloys

Time: Monday 15:45–17:00 Location: TC 006

MM 13.1 Mon 15:45 TC 006

Cluster expansions for kinetic Monte-Carlo simulations: towards time evolution with DFT accuracy — •Tobias C. Kerscher[1,2], Martin Leitner[1], Stefan Müller[2], and Raimund Podloucky[1] — [1]University of Vienna, Institute of Physical Chemistry, Vienna, Austria — [2]Hamburg University of Technology, Institute of Advanced Ceramics, Hamburg, Germany

We take first steps towards vacancy-mediated diffusion kinetics in aluminum alloys (e.g., Ni–Al and Fe–Al) by the combination of an ab initio based cluster expansion (CE) with Monte-Carlo simulations (MC). This method will incorporate many-body effects as well as variable transition barriers that depend on the structural environment of the jump, which is paramount for the calculation of MC jump rates according to transition state theory.

First, we present the energetics of selected transition paths in those Al alloys, determined by density functional theory (DFT) and the nudged-elastic-band method (NEB). Then, we show how the UNCLE code [1] and its kinetic Monte-Carlo algorithm will use a CE framework to include not only the energetics of all possible initial and final configurations of a transition, but also the correct configuration-dependent saddle points of the corresponding transition paths. Both contributions will be separately modeled by CEs based on ab initio input from DFT: the former by the energies of fully-relaxed input structures, the latter by the saddle points of the NEB method.

Work supported by FWF, Project number F4110 "ViCoM".

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

MM 13.2 Mon 16:00 TC 006

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

In order to reliably model the effects of both alloying and light elements within steels, it is essential to properly take into account the chemistry of the bonding between atoms, as well as the effects of charge transfer and magnetism. Density-functional theory provides such a reliable framework, but its computational expense places limitations on its applicability to large-scale and/or multi-component systems. The tight-binding approximation, including charge transfer and magnetism, can be derived directly from the Kohn-Sham energy functional. Since the electronic structure is obtained from a parametrised tight-binding Hamiltonian, the methodology offers an enormous computational advantage over ab-initio methods.

While many tight-binding models have obtained their parameters from density-functional calculations, they generally involve uncontrolled approximations for the matrix elements of the Slater-Koster Hamiltonian, which limits their transferability. The present work begins with the Harris-Foulkes energy functional, from which the parameters of the tight-binding model are obtained in a rigorous and umambiguous manner. We obtain transferable parametrisations of the environmental contribution to the tight-binding Hamiltonian and assess the validity of the approach by application to nickel-cobalt alloys.

MM 13.3 Mon 16:15 TC 006

Theoretical investigation of Cr-Sb compounds - structure and magnetic properties — •G. Kuhn[1], S. Mankovsky[1], S. Polesya[1], H. Ebert[1], M. Regus[2], and W. Bensch[2] — [1]Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany — [2]Christian-Albrechts-Universität, Institut für Anorganische Chemie, Max-Eyth-Straße 2, 24118 Kiel, Germany

We present a theoretical investigation of structural and magnetic prop-

erties of Cr-Sb compounds on the basis of ab-initio electronic structure calculations using the KKR Green's function method. Various compounds with different Cr:Sb ratio have been considered: Cr_3Sb in β-tungsten-structure, CrSb in NiAs-, NaCl-, Wurtzite- and Zincblende-structure and $CrSb_2$ in marcasite- and $CuAl_2$-structure.

The structural and magnetic stability have been analyzed performing total energy calculations. Magnetic properties of Cr-Sb compounds have been studied via Monte Carlo simulations based on the Heisenberg model with the exchange coupling parameters obtained by electronic structure calculations using the so-called Lichtenstein formula. This gives us both, the ground state magnetic structure of the compounds as well as their critical temperature which are found in rather good agreement with the experiment.

MM 13.4 Mon 16:30 TC 006

Effects of In concentration in $CuGa_{1-x}In_xSe_2$: a first-principles study — •Rolando Saniz, Dirk Lamoen, and Bart Partoens — Universiteit Antwerpen, Antwerpen, Belgium

Compounds of the family of $CuGa_{1-x}In_xSe_2$ alloys are of great current interest for the development of better absorbers for photovoltaic applications. To advance our understanding of the effects of alloying ratio, x, we carried out a state-of-the-art hybrid functional study of the structural and electronic properties of these materials for a series of x values. In contrast to previous theoretical results, we find that (i) the structural changes induced by increasing In content do not comply to Vegard's law, resulting in fact in a lowering of the symmetry of the system for intermediate In concentrations; (ii) as a function of x, the fundamental band gap does not follow a quadratic curve defined by a simple "bowing parameter"; (iii) the mixing enthalpies are very low and do not suggest any significant phase separation at finite temperatures.

MM 13.5 Mon 16:45 TC 006

Ground-state structures and elastic properties of Ni-Ti-Hf shape memory alloys: An ab-initio study — •Jürgen Spitaler[1,2], Daniel Lüftner[1,2], Rostam Golesorkhtabar[1,2], Peter Puschnig[2], and Claudia Ambrosch-Draxl[2] — [1]Materials Center Leoben Forschung GmbH, Rosegger-Strasse 12, 8700 Leoben — [2]Chair of Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben

Ni-Ti-Hf is a promising shape-memory alloy due to its higher Martensitic transformation temperature as compared to pure NiTi. In this transformation, the energetics and elastic behavior of different crystallographic phases play a crucial role. We have determined the stable phases of $NiTi_{1-x}Hf_x$ in the monoclinic structure (B19') as a function of the Hf concentration using the recently developed ATAT@WIEN2k interface. In order to improve the description of the disordered state, which is crucial for the quality of the expansion, special quasirandom structures were taken into account. We have determined the effective cluster interactions, based on the total energies of the fully-relaxed monoclinic supercells, which yields ordered groundstates for several Hf concentrations. The cluster expansion involves a rather high number of structures with positive formation energies, and it shows that Ti and Hf tend to form layers inside the unit cell. For the obtained groundstates we have determined the full elastic tensors and averaged macroscopic elastic properties structures applying ElaStic, a tool developed in our group.

MM 14: Topical Session Bulk Nanostrucured Materials III - Microstructure and Characterization I

Time: Monday 15:45–17:15 Location: H 0107

MM 14.1 Mon 15:45 H 0107

Absolute concentration of free volumes and related properties of ultrafine grained metals studied by time-dependent dilatometry — Bernd Oberdorfer[1], •Eva-Maria Steyskal[1], Wolfgang Sprengel[1], Michael Zehetbauer[2], Reinhard Pippan[3], and Roland Würschum[1] — [1]Inst. f. Materialphysik, TU Graz, Graz, Austria — [2]Physik Nanostrukturierter Materialien, Fak. f. Physik d. Universität Wien, Wien, Austria — [3]Erich Schmid Inst. of Materials Science, Leoben, Austria

Time-dependent dilatometry provides a direct approach to the absolute concentration of free volumes in nanophase materials, as it allows for a real-time observation of irreversible macroscopic length changes due to the annealing out of free volumes upon heat treatment. The ultrafine grained metals presented in this work were produced by severe plastic deformation via the high pressure torsion method. The annealing stages observed upon linear heating of severely plastically deformed iron, tantalum, copper, and nickel allow for an investigation of the absolute concentration as well as the kinetics of free volume type defects such as vacancies, dislocations, and grain boundaries [1]. Moreover a direct approach to the physical key parameter of specific grain boundary excess volume will be presented, using ultrafine grained nickel as a model system [2]. Financial support by the FWF Austrian Science Fund is appreciated (project P21009-N20).

[1] B. Oberdorfer et al., J. Alloys Comp. **509**, 309 (2011)

[2] E.-M. Steyskal et al., Phys. Rev. Lett, *in press*

MM 14.2 Mon 16:00 H 0107

Re-ordering of FeAl made nanocrystalline by high pressure torsion — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, 1090 Wien, Austria

In this work bulk intermetallic FeAl is made nanocrystalline by high pressure torsion deformation of a B2 ordered Fe-45at.%Al alloy. In the literature it was reported that in FeAl the long-range order is lost during deformation as indicated from X-ray measurements. In contrast, the present work shows that the disorder is not complete since it is revealed by TEM methods that chemically ordered nanodomains of about 2nm are observed after deformation [1]. Upon heating the long-range order is recurring by coarsening of the ordered nanodomains until they reach the grain size. Based on the coarsening of the chemically ordered nanodomains a model for the reordering process is developed and fitted to the results yielded from differential scanning calorimetry. This model allows to determine the vacancy concentration, the vacancy migration enthalpy and the vacancy migration volume. Finally, by annealing of specimens deformed by high pressure torsion without unloading, i.e. maintaining the hydrostatic pressure, their vacancy concentration is determined and compared to that after unloading. This leads to the result that vacancy relaxation occurs during unloading.

[1] C. Gammer, C. Mangler, H. P. Karnthaler, C. Rentenberger. Scripta Mater. 65, 57 (2011).

This work was supported by the Austrian Science Fund (FWF):[S10403,P22440].

MM 14.3 Mon 16:15 H 0107

High-pressure torsion induced open volume defects in Al-3wt%Cu investigated by positron annihilation spectroscopy — •Peter Parz[1], Michael Faller[2], Reinhard Pippan[2], Werner Puff[1], and Roland Würschum[1] — [1]Institut für Materialphysik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences and Department Materials Physics, University of Leoben, A-8700 Leoben, Austria

High-pressure torsion (HPT) has proven its capability to refine metals down to grain sizes of approximately 100nm [1]. In the case of age-hardenable aluminium alloys HPT deformation may significantly affect the process of precipitation hardening. In present work [2], an Al-3wt%Cu alloy was solution treated and quenched and subsequently subjected to HPT deformation. The defect structure and its annealing behaviour have been investigated by positron annihilation lifetime spectroscopy (PALS) and the chemical sensitive method of 2-dimensional Doppler broadening spectroscopy (2d-DB). Significant deviations of the mean positron lifetime and the chemical environment of the positron trapping sites due to HPT were detected.

[1] R. Pippan, F. Wetscher, M. Hafok, A. Vorhauer, I. Sabirov: The Limits of Refinement by Severe Plastic Deformation, Adv. Eng. Mater., 2006, 8, 11

[2] P. Parz, M. Faller, R. Pippan, W. Puff, R. Würschum: Microstructure and vacancy-type defects in Al-3wt%Cu after high-pressure torsion, Physics Procedia, accepted

MM 14.4 Mon 16:30 H 0107

DSC investigations on lattice defects in hydrogenated Pd processed by High Pressure Torsion — •Daria Setman, Maciej Krystian, Matthias Bönisch, Gerhard Krexner, and Michael Zehetbauer — Faculty of Physics, University Vienna, Austria

Disk-shaped Pd (99.95%) samples (diameter 6mm, thickness 0.8mm) were loaded with hydrogen in a Sieverts-type apparatus up to a hydrogen content [H]/[Pd]˜0.78. HPT-processing was performed at 195 K and 8 GPa hydrostatic pressure. DSC and TEM measurements revealed - for the first time - evidence of vacancy-hydrogen (Vac-H) clusters being formed during HPT. The vacancy densities from clusters reach atom concentrations as high as of order 10-3, and are thermally stable till 483 K (i.e. by 110 K higher than for undeformed Pd). Hydrogen desorption was monitored by microhardness and density measurements confirming effects typical of defect clusters on the mechanical properties. Results also demonstrate that hydrogen-assisted thermal stabilization not only occurs with vacancy-type defects but also with dislocations and grain boundaries, thus suggesting this effect for stabilization of nanocrystalline materials in general. However, prompt-gamma activation analysis showed that during annealing at RT for one year, the hydrogen desorbs completely, also including the part which had been trapped in the Vac-H-clusters.

[1] M. Krystian, D. Setman, B. Mingler, G. Krexner, M. J. Zehetbauer, Scripta Mater. 62, (2010) 49-52

Work supported by the Austrian Science Fund, Project S 10403

MM 14.5 Mon 16:45 H 0107

Self-similarity in junction controlled grain growth — •Dana Zöllner and Peter Streitenberger — Abteilung Materialphysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität, 39106 Magdeburg

The question of self-similarity in normal grain growth and particle coarsening has been a topic of research for decades, where statistical self-similarity was either found as an observation in experiments and simulations or used as an assumption for theoretical considerations. In the present work we show that self-similarity is also a feature of junction limited grain growth as it can be found in nanocrystalline materials. To that aim we analyse the influence of the various grain boundary junctions on grain growth kinetics by attributing to each type of boundary junctions an own specific energy and mobility resulting in nine types of growth kinetics each characterised by a self-similar scaling form of the growth law and corresponding self-similar grain size distribution function. In particular, for the cases of grain boundary, triple line and quadruple point mobility controlled grain growth the analytical model is in excellent agreement with the results of a modified Monte Carlo Potts model simulation based on a limited mobility of the boundary junctions.

MM 14.6 Mon 17:00 H 0107

Laser ultrasound for evaluation of microstructure of HPT nickel — Victor V. Kozhushko[1], •Heinz Krenn[1], and Reinhard Pippan[2] — [1]Karl-Franzens-University Graz, Graz, Austria — [2]Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria

The high pressure torsion (HPT) method is employed for grain size refinement of polycrystalline nickel. The grain structure of a disk specimen of about 30 mm diameter and 2.5 mm thickness is changed from coarse grains at the center to ultrafine grains (150 nm) at the periphery of the HPT-sample. The evaluation of the elastic properties was carried out by means of laser induced ultrasound. A noncontact sensor (5 mm pancake coil) based on an electromagnetic acoustic transducer (EMAT) and a permanent cylindrical magnet with the field of ˜0.25 T was attached to one side of the specimen. The coil detects the transient magnetic field due to the inverse magnetostrictive effect from the pressure pulse excited by the laser. The pronounced compression phase has nanosecond duration. The attenuation of the propagating ultrasound pulse is mainly due to the interaction with dislocations [1]. The scattering at grain boundaries produces longitudinal and shear waves which arrive to the sensor later than the primary pulse. Signals measured at different radii of the nickel specimen clearly showed a decrease of the ultrasonic attenuation with the HPT-refinement of the microstructure.

Financial support by the FWF Austrian Science Fund is appreciated (No. S10407-N16).

[1] V.V. Kozhushko et al., Key Eng. Mat. 465 (2011) 374

MM 15: Mechanical Properties III

Time: Monday 15:45–17:00 Location: H 0106

MM 15.1 Mon 15:45 H 0106

Microstructure and mechanical properties of γ' hardened Cobalt-base superalloys — •Steffen Neumeier, Alexander Bauer, and Mathias Göken — Institute I: General Materials Properties, University of Erlangen-Nürnberg, Germany

The material of choice for components in gas turbines like turbine blades and discs are Nickel-base superalloys. Due to their excellent mechanical properties, corrosion and oxidation resistance, they can bear high loads in harsh environments at high temperatures. The reason for the extraordinary mechanical strength at temperatures up to 80% of the melting temperature is the two-phase microstructure with a high volume fraction of the intermetallic γ' phase Ni_3Al ($L1_2$ crystal structure) coherently embedded in the γ phase, a face centered cubic Ni solid solution. Conventional solid solution and carbide hardened Cobalt-based alloys possess even a superior corrosion resistance, but they can be used only for low-loaded parts. In contrast to Nickel-base superalloys a similar γ/γ' microstructure, stable at high temperatures, could not be obtained in Cobalt alloys until the recent discovery of Sato et al. They found a stable γ' phase (Co_3(Al,W) with $L1_2$ crystal structure) in the ternary Co-Al-W system which has led to a new class of γ' hardened Co-base superalloys. In this paper the microstructure of several γ/γ' Co-base superalloys will be presented along with the mechanical properties at high temperatures. Creep experiments have shown that the creep strength is by far higher than that of conventional Cobalt based alloys and comparable to Nickel-base superalloys.

MM 15.2 Mon 16:00 H 0106

Modeling of anisotropic elasto-plastic material behavior with the phase-field method — •Daniel Schneider[1], Jan Höhn[2], Michael Selzer[1,2], Alexander Vondrous[2], and Britta Nestler[1,2] — [1]Institute for Applied Materials - Reliability of Components and Systems, Karlsruhe Institute of Technology — [2]Institute of Materials and Processes, Karlsruhe University of Applied Science

An extended phase-field model is formulated incorporating a formulation for elastic and anisotropic plastic effects ones on the evolution of microstructures. Thereby, the displacement field is computed by solving the local momentum balance dynamically. In order to calculate the plastic strain, a plasticity model is implemented consisting of an associated flow rule in combination with an anisotropic yield criterion and a linear hardening approximation.

Simulations with simple loads are performed illustrating the dynamic evolution of the stress and plastic strain in both, single phase systems as well as polycrystalline structures. Further, we present simulations of micro crack propagation induced by external forces with and without plastic deformations.

MM 15.3 Mon 16:15 H 0106

Theoretical study of dislocations in perovskite oxides — •Pierre Hirel[1,2], Matous Mrovec[1,2], and Christian Elsaesser[1,2] — [1]IAM-ZBS, Karlsruhe Institute for Technology, Engelbert-Arnold-Straße 4,76131 Karlsruhe (Germany) — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg (Germany)

Perovskite oxides such as barium-strontium titanate, lead zirconate-titanate, or potassium-sodium niobate are a technologically important and scientifically exciting class of materials. Many perovskites are ferroelectric and possess high dielectric constants, which make them attractive for modern microelectronic applications. A successful implementation however requires not only information about the intrinsic functional properties but also a thorough understanding of crystal defects that influence the functionality as well as the mechanical and structural stability of such components.

In the present work we investigate the properties of dislocations in perovskite materials by means of atomistic simulations, using both the

highly accurate first-principles calculations and computationally efficient classical interatomic potentials. We analyze the structures of dislocation cores in comparison to high-resolution transmission electron microscopy observations. The calculated Peierls energies and stresses for these dislocations under different applied loads give insight into their mobilities and are related to their macroscopic mechanical behavior.

(1) P. Hirel et al., Acta Mater. 60 (2012) 329

MM 15.4 Mon 16:30 H 0106

Mechanical spectroscopy and dislocation dynamics on Al_2O_3 particle reinforced Al-Mg-Si (AA6061) Alloys — •Jens Bernhardt and Hans-Rainer Sinning — Institut für Werkstoffe Technische Universität, Braunschweig, Germany)

Damping measurements using the vibrating-reed technique were carried out on an industrially used Al-Mg-Si (AA6061) alloys and also on 22 % Al_2O_3 particle-reinforced AA6061. Three different maxima in damping were found over a temperature range from 100 K to 800 K. Two damping peaks, located between 100 K and 400 K, are clearly related to the plastically deformed state of the material. Cold rolling of homogenized, unreinforced AA6061 gave rise to a broad damping peak with a visible substructure. In plastically deformed fcc metals, this peak is well known as Hasiguti Peak and is related to an interaction between dislocations, point defects and the crystal lattice. For the reinforced, homogenized and undeformed alloy a similar broad peak was observed after a subsequent heat treatment. In this case the microplastic deformation due to the misfit between the thermal expansion coefficient of matrix and the reinforcing particles is responsible for the emergence of the peak in damping. A further discussion of damping peak properties should reveal more detailed information about the underlying mechanisms and therefore about the influence of the reinforcing phase on dislocation dynamics.

MM 15.5 Mon 16:45 H 0106

Relaxor properties of pure and cerium doped calcium barium niobate — •Chandra Shekhar Pandey[1], Jürgen Schreuer[1], Manfred Burianek[2], and Manfred Mühlberg[2] — [1]Institute for Geology, Mineralogy and Geophysics, Ruhr-University Bochum, Germany — [2]Institute for Crystallography, University of Cologne, Germany

Lead-free relaxors Sr0.61Ba0.39Nb2O6 (SBN-61) crystallizing in the partially filled tetragonal tungsten bronze (TTB) structure types have attracted much interest because of their outstanding properties. Calcium barium niobate, CaxBa1-xNb2O6 (CBN-x), also belongs to the partially filled TTB structure family having high Tc at ~ 537 K. However, its relaxor behavior have not yet been reported.

We studied the elastic properties of pure and Ce doped CBN-28 (congruently melting; Czochralski grown) between 300K-1503K using resonant ultrasound spectroscopy. The relaxor phenomena for as-grown CBN single crystals was further explored by thermal expansion measurements, which revealed the characteristic temperatures Tb (Burns temperature, initiation of polar naonoregions PNRs), T* (temperature for first freezing of PNRs), and Tm at ~1100 K, ~800 K, and ~600 K, respectively [1]. These findings were confirmed by characteristic elastic anomalies. Cerium doping in pure CBN results in significant lowering of Tc and Tb; however, the intermediate temperature T* remains almost the same [2].

[1] C. S. Pandey, et. al., Phys. Rev. B 84, 174102 (2011). [2] C. S. Pandey, et. al., Appl. Phys. Lett. (Accepted).

MM 16: Microstructure and Phase Transformations I

Time: Monday 15:45–17:00 Location: H 1029

MM 16.1 Mon 15:45 H 1029

Deep liquid undercooling and nucleation in higher melting fcc metals — •Joachim Bokeloh, Marcel Heeger, and Gerhard Wilde — Institut für Materialphysik Münster

Since the melting enthalpy of fcc metals and therefore the driving force for crystallization scales with the melting temperature (T_m), one prediction of the classical nucleation theory (CNT) is that the onset of homogeneous nucleation for all fcc metals should be at about the same relative undercooling ($\Delta T/T_m$). While this was initially supported by experiments by Turnbull that showed a relative undercooling in the range of 0.17 to 0.18, the homogeneous nature of the nucelation was always questioned since CNT predicts a deeper undercooling before the onset of homogeneous nucleation. In a recent publication (PRL 107, 145701), new evidence was found that the crystallization of Nickel at a relative undercooling of 0.18 is indeed caused by homogeneous nucleation. Thus, the undercoolability of several fcc metals (Au, Cu, Co, Ni) is revisited by nucleation rate measurements with an heretofore unprecedented accuracy obtained by a statistical analysis of several thousand single crystallization events. Funding by the DPG (SPP1296) is greatfully acknowleged.

MM 16.2 Mon 16:00 H 1029

Crystallization behavior of an amorphous matrix with embedded heterogeneously distributed preexisting crystals: Geometric crystallization simulations and the Johnson-Mehl-Avrami analysis — •Martin Peterlechner[1], Thomas Waitz[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälische Wilhelms-University, Münster, Germany — [2]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Vienna, Austria

Nanocrystalline materials can be processed via crystallization of an intermediate amorphous phase. Controlling the grain size and thus the functional properties requires thorough knowledge of the kinetics of the crystallization processes. Probably the most widely applied kinetic model for crystallization reactions by nucleation and growth is the Johnson-Mehl-Avrami (JMA) model. The JMA model is analytical but based on rather strict assumptions such as a homogeneous distribution of nuclei with zero initial volume. To account for preformed heterogeneously distributed crystals that can strongly impact the crystallization behavior the present work focuses on simulations. A two-dimensional geometric model was used to systematically analyze the spatial distribution and initial volume fraction of preexisting crystals on the crystallization behavior. Using a constant nucleation and growth rate, it can be shown that with heterogeneously distributed preexisting crystals a bimodal structure after crystallization develops. The influence on the amount of heterogeneity and the number of preexisting crystals on the kinetic analysis using JMA is discussed.

MM 16.3 Mon 16:15 H 1029

Melting point depression of embedded Bi nano particles in Zn synthesized by rapid solidification — •Tae-Eun Song, Joachim Bokeloh, Martin Peterlechner, and Gerhard Wilde — Westfälische Wilhelms-Universität,Institute für Materialphysik, Wilhelmklemm-straße 10 D-48149 Münster, Germany

The melting point depression of embedded Bi nano particles in a Zn matrix synthesized by rapid solidification was analyzed using Differential scanning calorimetry (DSC), Scanning electron microscope (SEM) and Transmission electron microscopy (TEM). SEM and TEM results reveal the Bi particle size distribution of the as prepared state and after annealing at the relevant temperature. DSC results reveal the embedded Bi particles are solidified at two different undercooling levels. Some Bi particles are solidified at a small undercooling with a number of exothermic peaks. Other Bi particles are solidified with a broad exothermic peak at a larger undercooling level. During repeated heating and cooling through the early melting peak, the enthalpy for solidification gradually decreases. The possible explanations based on thermodynamics or based on coarsening kinetics will be discussed.

MM 16.4 Mon 16:30 H 1029

Effect of quenching rate on the clustering behavior of Al-Mg-Si alloys — •yong yan[1], meng liu[1,2], cynthia chang[1], julian kühn[1], and john banhart[1,2] — [1]Technische Universität Berlin, Materials Science and Technology, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz Center Berlin for Materials and Energy, Applied Materials, Hahn-Meitner-Platz, 14109 Berlin, Germany

In order to investigate the effect of quenching rate on the clustering kinetics during natural aging (NA), high purity Al-Mg-Si alloys are quenched to different temperature and media. In-situ Positron Annihilation Lifetime Spectroscopy (PALS) and In-situ resistivity mea-

surements at room temperature were then performed. It is found that four stages of changes in positron lifetime are directly observed. The quenching rate influences the first decrease of the lifetime during NA. The influence is larger for samples with lower solute content. On the other hand, a first decrease in the resistivity is observed in all alloys before the increase that is due to clustering of solute atoms. The amplitude of the decrease is more significant for samples with lower solute content and lower quenching rate. The first decrease in the positron lifetime and resistivity is discussed in terms of the interaction of vacancy and solute atoms.

MM 16.5 Mon 16:45 H 1029

Solidification along liquid-liquid interfaces in syntectic systems — •Claas Hüter[1], Guillaume Boussinot[1,2], Efim Brener[2], and Robert Spatschek[1] — [1]MPIE, Düsseldorf, Germany — [2]PGI, Forschungszentrum Jülich, Germany

Syntectic transformations belong to transitions which exhibit three-phase equilibria in binary alloys, and we consider solidification along the interface in undercooled demixed liquids. The formulation of the steady-state problem is obtained in terms of boundary integrals . The focus of our investigation is on the scaling relations which we obtain in the regime of small deviations from solutions which show symmetric interface shapes.

MM 17: Poster Session

Time: Monday 17:00–19:00 Location: Poster B

MM 17.1 Mon 17:00 Poster B

Oxidation of monovacancies in graphene by oxygen molecules — Thaneshwor Kaloni, Yingchun Cheng, and •Udo Schwingenschlogl — 4700 King Abdullah University of Science and Technology Thuwal 23955-6900

We study the oxidation of monovacancies in graphene by oxygen molecules using first principles calculations. In particular, we address the local magnetic moments which develop at monovacancies and show that they remain intact when a molecule is adsorbed such that the dangling carbon bonds are not fully saturated. The observed value of magnetic moment is 1.35 Bohr Magneton for monovacancy and it becomes 1.86 Bohr Magneton by oxygen adsorption on monovacancy in graphene. However, the lowest energy configuration does not maintain dangling bonds and is found to be semiconducting. Our data can explain the experimentally observed behavior of graphene under exposure to an oxygen plasma.

MM 17.2 Mon 17:00 Poster B

Thermal stability and crystallization of magnetron sputtered amorphous Si2C — •René Gustus[1,2], Wolfgang Gruber[2], Lienhard Wegewitz[1,3], Harald Schmidt[2,3], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Straße 42, Clausthal-Zellerfeld, Germany — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

During the last decades, amorphous silicon carbide (SiC) has attracted much attention in several fields of scientific research. Non-stoichiometric amorphous SiC became of specific interest due to the possibility of tailoring the material properties by varying its chemical composition. We investigated the thermal stability and the crystallization of magnetron sputtered amorphous non-stoichiometric Si2C deposited on silicon substrates, by means of XPS, AES, XRD, AFM and SEM. Crystallization of amorphous Si2C takes place at temperatures around 800 °C, accompanied by the growth of silicon crystalls on the surface. Annealing at 1200 °C for 2 hours leads to crystallization of silicon and silicon carbide, coupled with the formation of large structures and a silicon enrichment in the surface region of the film. After 20 hours of anealing at 1200 °C, the crystalized silicon has disappeared from the surface and no silicon enrichment is detectable any longer. The experimental results and the underlying processes are discussed.

MM 17.3 Mon 17:00 Poster B

Atomistic study of the elastic properties of alpha' martensite crystals — •Nina Gunkelmann and Herbert M. Urbassek — Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern

Material phycisists have long-standing experience in modeling of pure iron by atomistic simulations. There exist a number of interaction potentials describing the properties of this material. In contrast, only a few interatomic potentials have been developed for the iron-carbon system; these have not yet been fully characterized with respect to the mechanical properties of martensitic crystallites. This seems surprising because of the high-technologic importance of steel. In this work the elastic properties of iron-carbon crystals are characterized using molecular dynamics simulation and compared with available experimental data.

MM 17.4 Mon 17:00 Poster B

Measurement of nucleation rates using fast scanning calorimetry on samples prepared by the Droplet Emulsion Technique (DET) — •Christian Simon, Joachim Bokeloh, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The most difficult part in heterogenous nucleation experiments is the control of the heterogenous nucleant. On one hand, parasitic nucleants like the container wall and impurities must be removed, and on the other hand the target nucleant phase must be kept at a constant potency. The DET is uniquely suited to accomplish this task. With the DET microsized droplets of a material are prepared by heating it above the melting temperature in a special organic solution and then dispersing it to a fine emulsion of droplets by violent stirring. While the fine dispersion reduces the influence of impurities, the organic solution forms a non-catalytic surface layer and thus reduces the nucleation potency of the surface.

The nucleation rate is evaluated by a statistical analyses that treats nucleation as a non-homogenous Poisson process. A DSC measurement is used to analyse the undercooling of an ensemble of droplets. A fast scanning nano-calorimeter (10 K/s - 100000 K/s) is used to analyse the undercooling and nucleation rate over a large number of repeated heating-cooling-cycles on single droplets, allowing for an heretofore unprecedented accuracy in the nucleation rate measurement.

MM 17.5 Mon 17:00 Poster B

New deposition concept for the precise tailoring of nanocomposites with a gas aggregation cluster source — •Björn Gojdka[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Viktor Hrkac[2], Jian Xiong[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Institute for Materials Science (Multicomponent Materials), Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, D-24143 Kiel, Germany — [2]Institute for Materials Science (Synthesis and Real structure), Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, D-24143 Kiel, Germany

Nanocomposites with embedded magnetic particles are of special interest due to their unique properties which are, for example, highly relevant for data storage or high-frequency applications. However, in order to tailor a nanocomposite for a certain application, advanced process control is necessary. In addition, during deposition most magnetic materials react with a non-inert process atmosphere or the matrix constituents, thus degrading the ferromagnetic properties of the nanoparticles in the composite. We present a new concept for the precise tailoring of a wide variety of nanogranular composites based on a modified co-sputtering concept with a gas aggregation cluster source. To demonstrate the feasibility of the concept, magnetic cobalt nanoparticles are embedded in a dielectric matrix. Subsequently, the chemical, magnetic and structural properties of the composite were investigated by energy dispersive x-ray spectroscopy, vibrating sample magnetometry and transmission electron microscopy.

MM 17.6 Mon 17:00 Poster B

Nonlinear response of metallic glasses at high applied stresses and nonlinear effects of damping behaviour below to above the glass transition temperature — •Antje Krüger, Moritz Schwabe, and Konrad Samwer — I. Physikalisches Institut, Uni-

versität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The α- and β-processes in metallic glasses can be described within the model of the potential energy landscape (PEL). These processes illustrate barriers for a change of local configurations and can be varied by external stresses. When applying a constant stress the sample responds in a combination of different behaviours, elastic, anelastic and plastic.

In the previous work we studied the anelastic contribution in order to obtain information about the damping behaviour. The results showed an exponential correlation to temperature and stress [1]. Now, we also can estimate the activation volume of the α- as well as the β-process using these creep-recovery-methods [2]. Furthermore we investigate in the viscous flow the Newtonian and non-Newtonian behaviour when increasing the elastic strain σ_0/E. This can be compared to well known results in polymers, granular and colloidal systems. Work supported by FOR1394 and GRK782.

[1] M. Schwabe, D. Bedorf and K. Samwer, The European Physical Journal E (2011), 34, 91

[2] M. Schwabe, S. Küchemann, H. Wagner, D. Bedorf and K. Samwer, Journal of Non-Crystalline Solids (2010), 357, 490-493

MM 17.7 Mon 17:00 Poster B

Ab-Initio Hamiltonian and Hedin's Equations for Phonon-Induced Effective Electron-Electron Interaction — •Ronald Starke — Department of Computational Materials Physics, Uni Wien, Sensengasse 8/12, A-1090 Wien, Austria

Ab-initio methods are usually applied to electronic structure theory with an electron-electron interaction given by the Coulomb potential. Nonetheless, it is well-known that the nuclear degrees of freedom (regrouped as phonons) lead to a broad range of effects from modifications in the optical spectra up to superconductivity. On a fundamental level, the phononic degrees of freedom constitute a physical system in its own right. Hence, the total system cannot be described by a purely electronic Hamiltonian. As a first approximation, one disregards the phononic degrees of freedom by taking them into account through an effective electron-electron interaction. This gives rise to a huge field of effective models, the most prominent being BCS theory. However, these effective models clearly do not match the standards of ab-initio electronic structure calculations: not only is the effective phonon-induced electron-electron interaction not parameter free, even worse, important ingredients of the fundamental ab-initio electronic Hamiltonian like the Coulomb potential are not taken into account. We review how this problem can be overcome by the addition of an phonon induced effective but ab-initio electron-electron interaction to the standard ab-initio Hamiltonian and discuss the corresponding modified Hedin equations.

MM 17.8 Mon 17:00 Poster B

Diffusion and microhardness in ultrafine grained nickel — •Simon Trubel, Sergiy Divinski, Gerrit Reglitz, Jörn Leuthold, and Gerhard Wilde — Westfälische Wilhelms-Universität, Institut für Matrialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

Ultrafine grained and nanocrystalline materials produced by methods of severe plastic deformation have roused a growing interest in science and technology. To determine how certain characteristics of internal interfaces in a material are affected by severe deformation, diffusion is a suitable method. The material under investigation is nickel in a purity of 99.6%. High pressure torsion (HPT) is applied where nickel discs are subjected to quasi-hydrostatic pressure of 2 GPa and torsionally deformed several times. Ultrafine grained Ni is produced and grain boundary self-diffusion is measured at several temperatures applying the radioactive isotope 63Ni. The HPT process refines the grain size in the material and the grain boundary diffusion is significantly enhanced. Nanoindentation is used to obtain information about mechanical properties of the material and their evolution with annealing temperature.

MM 17.9 Mon 17:00 Poster B

From structure refinements of ε-Al–Pd–Mn phases toward decagonal quasicrystals — •Benjamin Frigan[1], Marek Mihalkovič[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

We have studied and resolved occupancy correlations in the existing average structure model of the complex metallic alloy ξ'-Al–Pd–Mn, which has approximately 320 atoms in the unit cell and many fractionally occupied sites. Model variants were constructed systematically in a *tiling-decoration approach* and subjected to simulated annealing by use of both density functional theory and molecular dynamics with empirical potentials.

The main structural building blocks of ξ' are pseudo-Mackay icosahedral (PMI) clusters which form columns parallel to (0,1,0) and when projected are vertices of a hexagonal tiling. The tiling representation allows to extend structure models for the ξ'-phase to structure models of other closely related phases where the projections of the PMI columns also form pentagon and nonagon tiles. Our refined tiling-decoration model applies to any structure within the so-called ε-phases family.

We further extend our tiling-decoration model and present a detailed atomistic description of all tiles that are observed in the decagonal quasicrystalline phase. We show how aspects of both the ε-phases and the decagonal phase can serve as a starting point for an accurate microscopic modeling of the *metadislocations*.

MM 17.10 Mon 17:00 Poster B

Investigation of stable intermediate states in fourfold nanosystems — •Andrea Ehrmann[1] and Tomasz Blachowicz[2] — [1]Hochschule Niederrhein, Faculty of Textile and Clothing Technology, Mönchengladbach, Germany — [2]Institute of Physics, Silesian University of Technology, Gliwice, Poland

In systems of four crossed ferromagnetic nano-wires, pronounced magnetization steps in the hysteresis loops have been found using micromagnetic simulations [1]. The steps can be attributed to stable intermediate states, similar to flux-closed vortex states in ferromagnetic nano-rings.

Due to the fourfold anisotropy of the system of four coupled nanowires, these states can be distinguished even by measuring the magnetization of the whole system, giving rise to four separated states in the absence of an external magnetic field. Opposite to actual trials with nano-rings or layered structures, no additional method of symmetry breaking is necessary. Downscaling the system leads to qualitative changes in the magnetization reversal, which have to be taken into account by changing the material or adjusting the design.

Such a system can be utilized, e.g., in quaternary (four states, i.e. two bits per magnetic nano-object) magnetic storage applications.

[1] T. Blachowicz, A. Ehrmann: Fourfold nanosystems for quaternary storage devices, J. Appl. Phys. 110, 073911 (2011)

MM 17.11 Mon 17:00 Poster B

Design and Operation of a Nano-Calorimeter for high Sensitive and Fast heating rates measurements — •Mostafa Mohamed, Joachim Bokeloh, Tae-Eun Song, and Gerhard Wilde — Institute of Materials Physics, Westfalische Wilhelms University Muenster,Muenster,48148,Germany

A thin-film differential scanning calorimetric (TDSC) technique has been developed based on Silicon-Nitride (Si-Nx) membranes, for use as a Nano-calorimeter detector in high-sensitivity measurements. The Nano-calorimeter is specifically designed to determine the thermal properties and heat capacity of nano-structured materials, with very high sensitivity values and fast heating rates (104 K/S). The (Si-Nx) membrane was used as a low thermal mass mechanical support structure. The measurements of the system are accomplished via electrodes of Pt or Au that are used for resistive heating and resistive temperature measurement simultaneously. The method shall be applied first to measure the melting of various amounts of pure evaporated metal thin films.

MM 17.12 Mon 17:00 Poster B

Direct Single Electron Imaging with a pnCCD for TEM — •Henning Ryll — PNSensor GmbH, München

Promising better resolution and sensitivity, work on a spatially resolving direct electron detector, based on a pnCCD is presented.

A pnCCD is a back-illuminated silicon detector, which is sidewards depleted. By applying appropriate voltages to both sides, the whole 450 um thick bulk, high-purity n-type silicon is depleted.

Up to 1000 full frames per second are achieved, enabling the imaging of single electrons in ultra-low dose modes and the observation of changes in samples. Each electron creates a signal easily distinguished from the noise. The final image is obtained by successive addition of individual frames and their intensities. Additionally image processing at the single incident electron level and its signal can be performed.

In order to determine the characteristics of the pnCCD, one type

with a pixelsize of 51x51um^2 was tested on a Phillips CM12 120 keV TEM. A slanted knife edge was placed in front of the detector to determine the MTF. Operating at 120 keV and a low dose, applying signal processing allowed for a software subpixel resolution, improving the MTF to >40% @ Nyquist.

Simulations complementing the experimental data will be presented, as well as the expected pixel patterns and their analysis for different energies.

MM 17.13 Mon 17:00 Poster B

Investigation of strain fields along shear bands in a deformed Pd40Ni40P20 bulk metallic glass — •Severin Schlottbom, Jonas Bünz, Jörn Leuthold, Stefan Ostendorp, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Plastic deformation of metallic glasses induces shear bands, which form quasi-instantaneously once a critical loading is exceeded. The mechanism of deformation is essential for the mechanical properties of amorphous metals, but not deeply understood yet. The knowledge of strain fields along a single shear band might provide access to understanding the basic deformation mechanism of the shear transformation zones (STZ) forming the shear bands. In this work the initiation of shear bands and their influences on the adjacent unaltered matrix is investigated. Undeformed Pd40Ni40P20 bulk metallic glass was coated with gold nanodots by PVD, delivering a nanoscale grid, which is used to monitor the strain fields during shear deformation. The as-cast and subsequently cold-rolled samples were examined by scanning electron microscopy and digital image correlation is used in order to determine the strain fields.

MM 17.14 Mon 17:00 Poster B

Generation of force field for molecular dynamic simulations of zirconia — •Andreas Irmler, Philipp Beck, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik (ITAP) , Universität Stuttgart

We have generated force fields for crystalline and molten metal oxides. With these force fields, we intend to simulate microstructural and thermodynamic properties of systems with millions of atoms. We use DFT calculations to obtain forces, stresses and energies of reference systems with several hundred particles. Via potfit [1], a force matching package, we generate interaction potentials by adjusting its parameters to optimally reproduce the reference data computed in ab-initio calculations. We use Wolf summation [2] to handle long range electrostatic interactions. This direct, pairwise summation method scales linearly in the number of particles. The polarizability of oxygen atoms is described with Tangney-Scandalo [3] force field model. With this approach we have created force fields for several metal oxide systems in liquid and solid state. These force fields were tested in molecular dynamic simulations and show good agreement with experimental results. In the present contribution, we show the application to crystalline zirconia.

[1] P.Brommer *et al.*, Modelling Simul.Mater.Sci.Eng. **15** ,295 (2007).
[2] D. Wolf *et al.*, J. Chem. Phys. **110**, 8254 (1999).
[3] P. Tangney and S. Scandalo, J. Chem. Phys. **117** 8898 (2002).

MM 17.15 Mon 17:00 Poster B

Order-disorder transformation in copper-gold alloys revisited by in situ X-ray diffraction — •Max Metelmann, Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institute of Materials Physics, Wilhelm-Klemmstr. 10, 48149 Münster, Germany

CuAu alloys with an equi-atomic composition exhibit a well known order-disorder phase transformation in the solid state. Detailed analyses of this order-disorder transition were performed using in situ heating X-ray diffraction.This method enables temperature and time-resolved studies of the long range order parameter, which can be calculated from diffraction spectra. By means of in-situ X-ray diffraction, the temperature dependence of the peak intensity has been investigated, i.e. the Debye-Waller factor has been determined. In addition, the decrease of the peak intensity with increasing temperature and increasing angle of incidence is modeled. The comparison between experiments and calculations indicates that the experimental results are imprecisely described. The results are discussed with respect of corrections to the theoretical description of the Debye-Waller factor.

MM 17.16 Mon 17:00 Poster B

Finite element based fatigue predictions for Thermal-Acoustical-Protective-Shields — •Martin Kollenrott and Othmar Marti — Department of Experimental Physics, Ulm University

In the engine compartment more and more temperature-sensitive parts are being used. Thermal-Acoustical-Protective-Shields (TAPS) protect these parts from high temperature impact. TAPS are exposed to different periodic forces and temperatures mainly induced by the engine. The subject is to guaranty the lifetime resistance against fatigue of the part. In the ongoing project a finite element based model for fatigue of TAPS has to be developed.

To predict durability, dynamic and forming stresses are important. For a dynamic stress prediction it is necessary to determine loss factors for the 3-D formed thin sheet metal layers. These measurements are performed with a laser-vibrometer with impulsive or vibratory excitation of the parts. To determine forming stresses, finite element based forming simulations are performed. A Woehler curve depending on the pre-stressed material at the previous forming process is used for every node in the finite element mesh to predict cracks.

MM 17.17 Mon 17:00 Poster B

Ab initio and kinetic Monte Carlo modelling of Fe-Cu-Ni-Mn alloys — •Stephen Hocker, Peter Binkele, Alejandro Mora, and Siegfried Schmauder — Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Universität Stuttgart

Formation and growth of precipitates in thermally aged Fe-Cu-Ni-Mn alloys at temperatures above 573 K is investigated by kinetic Monte Carlo simulations. A thermally activated vacancy diffusion mechanism on a rigid bcc lattice is used to characterize the processes of nucleation and growth of Cu clusters. Important input parameters for the Monte Carlo simulations are mixing energies and vacancy formation energies. DFT based ab initio calculations are presented which provide these data. Monte Carlo simulations are performed with a thermodynamically based set of input parameters as well as with the ab initio based set of parameters. It is shown that the Monte Carlo results are very sensible regarding these input data. The influence of the Ni and Mn atoms in the precipitation of Cu rich clusters is analyzed for both simulation setups.

MM 17.18 Mon 17:00 Poster B

Synthesis and electrochemical properties of tailored $LiMPO_4$ (M= Mn, Co) — •Christoph Neef, Carsten Jähne, and Rüdiger Klingeler — Kirchhoff Institut für Physik, Universität Heidelberg, Germany

Due to their high stability and theoretical capacity, transition-metal olivine phosphates offer a large potential for application as positive electrodes in Li-Ion batteries. Among $LiFePO_4$, which is already used in high power cells, $LiMnPO_4$ and $LiCoPO_4$ are interesting compounds because of their high open cell voltage vs. Lithium of 3.9V and 4.6V respectively. Here we report on the microwave assisted hydrothermal synthesis of $LiMnPO_4$ and $LiCoPO_4$ and their electrochemical characterisation by means of cyclic voltammetry and impedance spectroscopy. Variation of synthesis parameters as well as wet ball milling are used for size and shape tayloring of the particles. PEIS is used to study the morphology influence on high and low frequency impedance and thus on charge transfer resistances, ion diffusion and double layer capacitances. We found that size reduction of particles increases the electrochemical performance, however the extensive application of ball milling may cause a loss of crystal structure and thus reduces the ability of lithium intercalation / deintercalation.

MM 17.19 Mon 17:00 Poster B

Phason flips in quasicrystals: Interpretation of HRTEM data 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, this process is very slow, flips occur in periods of seconds or even minutes.

On the one hand, we analyze the temporal evolution and statistical properties of the spots shown on HRTEM images provided by K. Edagawa. On the other hand, we perform kinetic Monte Carlo simulations [2], using several statistical model systems, e.g. based on a structure

model for d-Al-Cu-Co suggested by Zeger et al. [3]. There rings of ten atoms can perform flips by collective motion of atoms inside decagonal double layers.

We relate the experimental data to our simulation results, and demonstrate how flip frequencies depend on the number of decagonal layers and on the strength of their interaction.

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

MM 17.20 Mon 17:00 Poster B

Atomistic simulation of severe plastic deformation-induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinsky[1], Anatha Padmanabhan[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Münster — [2]University of Hyderabad, India

A comparison of microstructures, properties and transport kinetics in materials subjected to the last stages of severe plastic deformation (SPD) or steady-state superplastic flow indicates a number of unexpected similarities especially with respect to the interface response on the deformation, such as formation of an interface hierarchy, deformation localization, grain boundary sliding events when dislocation activities are suppressed, etc. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle grain boundaries in SPD-processed materials in terms of the concept of shear localization in the interfaces and choosing oblate spheroids as basic units of sliding.

"Non-equilibrium" grain boundaries in Cu are simulated. The individual simulation steps include generation of a grain boundary; determination of regions corresponding to the oblate spheroids on the boundary plane; introduction of an extra free volume (a fraction of atoms in the oblate spheroids is simply deleted) and shearing of the oblate spheroids by a given amount. By energy minimization, a high-energy state of the grain boundary is found which corresponds to about 4% additional free volume and 0.1 unit shear. The subsequent response of such an interface on the applied shear is analyzed.

MM 17.21 Mon 17:00 Poster B

Towards kinetic Monte-Carlo simulations with ab initio accuracy — •Martin Leitner[1], Tobias C. Kerscher[1,2], Stefan Müller[2], and Raimund Podloucky[1] — [1]University of Vienna, Institute of Physical Chemistry, Vienna, Austria — [2]Hamburg University of Technology, Institute of Advanced Ceramics, Hamburg, Germany

For the Ni–Al and Fe–Al alloy system we present the first steps towards kinetic Monte-Carlo (KMC) simulations with ab initio accuracy. Many body interactions which describe the energetics of both the local minima and migration states are included by cluster expansions (CE) in the framework of the UNCLE code [1].

In this model approach single atoms jump to vacant nearest-neighbor sites and have to overcome configuration dependent migration barriers. According to transition state theory (TST) jump rates are then derived by the energy difference between initial and saddle point state. The KMC simulations require a) vacant lattice sites, which enforce a ternary CE for a binary compound, and b) the configuration dependent height of the saddle points, which have to be calculated and included in the CE.

We discuss different aspects of jump profiles in the respective systems computed by density functional theory (DFT) calculations.

The support of FWF project 4110 (ViCoM) is acknowledged.

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

MM 17.22 Mon 17:00 Poster B

Interactions in Fe-Pd — •Cédric Sax and Bernd Schönfeld — LMPT, Department of Materials, ETH Zurich

X-ray diffuse scattering was measured from single-crystalline Fe-80 at.% Pd. A state of thermal equilibrium - corresponding to 1073 K - was investigated at room temperature. Maxima of diffuse scattering were found at X positions. Short-range order scattering was separated by the Georgopoulos-Cohen technique and effective pair interaction (EPI) parameters were determined by the inverse Monte Carlo method. In contrast to the set of EPI parameters that were obtained by Mehaddene et al. for Fe-50 at.% Pd, a dominant and positive value for the nearest-neighbor interaction is now found. This outcome indicates a stronger ordering tendency for Fe-Pd with a higher Pd fraction. Using linear interpolation between the EPI parameters at both compositions, shifts in the highest order-disorder transition temperatures of the $L1_0$ and $L1_2$ phases away from stoichiometry are obtained. Direct experiments confirm these findings.

MM 17.23 Mon 17:00 Poster B

Structure and thermal stability of severely plastically deformed Cu84Al16 — •Nazar Ibrahim, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University Münster,Germany

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

MM 17.24 Mon 17:00 Poster B

Tuning of the silver ion release from polymer-metal nanocomposites containing gold-silver alloy or gold-core/silver-shell nanoparticles — •Nisreen Alissawi, Irmak Kocabas, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — Institute for Materials Science - Multicomponent Materials, Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiser Str. 2, 24143, Kiel, Germany

The tuning of silver ion release could be important for antimicrobial applications of silver where a controlled release is desired to prevent e.g. damage of human cells. Two dimensional Au-Ag alloy or Au-core/Ag-shell nanoparticle ensembles with various compositions on PTFE were prepared by physical vapor deposition (PVD) techniques and silver ion release kinetics in water were studied by determination of the dissolved silver using atomic absorption spectroscopy (AAS). Changes in the morphology, optical properties and composition of the nanocomposites were examined by using transmission electron microscopy (TEM), UV-visible spectroscopy (UV-Vis) and X-ray photoelectron spectroscopy (XPS), respectively. Results indicate that with increasing the gold fraction in the Au-Ag alloy nanoparticles a strong improvement of the oxidation resistance of the AgNPs occurs. This can be a good way to control the release of silver ions in solutions. Moreover, the effect of a polymer barrier of certain thickness was investigated for both model systems and the silver ion release rate was slowed down.

MM 17.25 Mon 17:00 Poster B

Cooling rate dependence of undercooling of pure Sn single partially molten drop by fast scanning calorimetry — •Bin Yang[1], Alexander Sasha Abyzov[2], Evgeny Zhuravlev[1], Yulai Gao[3], Jürn W. P. Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]National Science Center, Kharkov Institute of Physics and Technology, 61108 Kharkov, Ukraine — [3]Shanghai Key Laboratory of Modern Metallurgy & Materials Processing, Shanghai University, Shanghai 200072, P.R. China

The partial melting of a pure Sn single micron sized particle is successfully performed by non-adiabatic differential fast scanning calorimetry. In a large range of cooling rates spanning three orders of magnitude solidification undercooling is observed for the partially molten particle. The cooling rate dependence of undercooling is correspondingly investigated. Our data indicate that the kinetics of nucleation changes with decreasing cooling rate. The differential fast scanning calorimetry opens up the possibility to experimentally study the kinetics of nucleation and growth processes of single metallic particles at rapid solidification extending the theoretical analysis of these processes performed in previous studies.

MM 17.26 Mon 17:00 Poster B

Texture gradient in ultrafine-grained Ti/Al composite wires produced by accumulative swaging and bundling — •Andy Eschke[1], Juliane Scharnweber[1], Carl-Georg Oertel[1], Tom Marr[1,2], Jan Romberg[1,2], Jens Freudenberger[2,3], Uta Kühn[2], Ludwig Schultz[1,2], Jürgen Eckert[1,2], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, Germany — [2]Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [3]Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, Germany

Various top-down processes of severe plastic deformation (SPD) like equal channel angular pressing, high pressure torsion or accumulative roll bonding are well known for producing ultrafine-grained (ufg) microstructures. The evolution of texture with respect to deformation by an alternative SPD process, called accumulative swaging and bundling (ASB), is shown for ufg Ti/Al wires, suitable for structural materials because of their high specific strength. An Al rod was stacked into a Ti tube and swaged with an area reduction of approximately 20% per pass to a logarithmic strain of 4.3. The resulting composite wire was cleaned, cut into 37 pieces, stacked into a Ti tube (of initial dimension) in a hexagonal arrangement and then swaged again. This procedure can be repeated arbitrarily. The texture gradient of the ASB composites was studied using a X-ray micro diffraction system D8 DISCOVER (Bruker AXS GmbH) equipped with a micro focus X-ray tube IμS and an area detector Vantec-2000. The results will be discussed with respect to processing and grain refinement.

MM 17.27 Mon 17:00 Poster B

Phase Field Simulations of Martensitic Transformation in Thin Films — •Alexander Auge, Niclas Teichert, and Andreas Hütten — Bielefeld University, Department of Physics, Universitätsstr. 25, 33615 Bielefeld, Germany

Magnetic shape memory materials like Ni-Mn-Ga and Ni-Mn-Sn have been intensively investigated in the past few years due to their potential applications in magnetic cooling or actuators. The physical origin of these effects is the martensitic transformation (MT) in combination with ferromagnetism. For many applications, like magnetic cooling, thin films are advantageous or even mandatory. The confinement due to the film thickness and also the constraint of the substrate can have a major influence on the transition and even hinder a MT completely. To understand what the major contributions to the change in the MT are and how to optimize the performance of the MT in thin films, phase field simulations are carried out. A three dimensional Landau theory for multivariant phase transformations developed by Levitas et al. [1] is used in the framework of finite element simulations. The most relevant energy contributions in dependence of film thickness and the resulting microstructure are presented.

[1] V. I. Levitas and D. L. Preston, Phys. Rev. B 66, 134207 (2002)

MM 17.28 Mon 17:00 Poster B

X-ray diffraction studies on low alloyed and high-Mn steels with TRansformation and TWinning Induced Plasticity (TRIP, TWIP) — •Andre Steffen[1], Hendrik Quade[2], Raphael Twardowski[2], Sascha Buthmann[2], Michael Paulus[1], Christian Sternemann[1], Ulrich Prahl[2], Wolfgang Bleck[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, D-44221 Dortmund. — [2]Institut für Eisenhüttenkunde, RWTH Aachen, D-52072 Aachen.

High manganese austenitic steels and low alloyed TRIP steels combine high strength and formability. Therefore they get high attention regarding the applications in automotive parts and safety-sensitive areas. The excellent mechanical properties of these steels result from different deformation mechanisms, such as the martensitic transformation and twinning. The TRIP and TWIP effect does not only result in an increase in hardening but also postpones necking or damage to later deformation degrees, which leads to a better formability. For the investigation of the TRansformation Induced Plasticity effect during straining several commercial low-alloyed TRIP steels were analysed. The investigations were carried out in-situ using a tensile testing machine. Further investigations on high-Mn steel tensile TWIP samples with varying microstructure were performed. The microstructure was set by annealing and quenching. Afterwards the samples were prestrained to 5 %, 10 %, 20 %, 30 % and 40 % of true strain. The tensile tests were carried out for a temperature range of 123 K to 423 K and a strain rate of 0,004 s^{-1}.

MM 17.29 Mon 17:00 Poster B

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

Lithium titanate (LTO) is used as an anode material in lithium ion batteries, as it reveals both, electronic as well as Li-ion conductivity. Both conductivities and the capability to reversibly intercalate/deintercalate lithium, strongly depends on the lithium diffusivity of the material, which is difficult to obtain in case of powder material, because of its porous structure. Therefore, due to their well defined structure and the absence of e.g. conductive binder, ion-beam sputtered thin film electrodes of LTO are appropriate for diffusion studies, as they give access to the diffusivity of lithium in pure LTO. In this work we prepared thin films of LTO by reactive rf-ion beam sputtering and carefully proofed the structure of the films by X-ray diffraction and transmission electron microscopy. Afterwards, we applied galvanostatic intermittent titration technique (GITT) technique to determine the chemical diffusion coefficient, i.e. by evaluating the electrical potential of the LTO layer vs. lithium, when applying a pulsed current signal. Due to the thin film geometry of our samples, it was possible to reliably evaluate the GITT results by assuming the thin approach and to obtain the lithium diffusivity in LTO as a function of the lithium concentration.

MM 17.30 Mon 17:00 Poster B

Electrochemical tuning of the electrical resistance of nanoporous platinum produced by dealloying — •Eva-Maria Steyskal[1], Maximilian Besenhard[1], Thomas Traussnig[1], Jörg Weissmüller[2], Stephan Landgraf[3], and Roland Würschum[1] — [1]Inst. f. Materialphysik, TU Graz, Graz, Austria — [2]Inst. f. Werkstoffphysik u. Werkstofftechnologie, TU Hamburg-Harburg, Hamburg, Germany — [3]Inst. f. Physikalische u. Theoretische Chemie, TU Graz, Graz, Austria

Nanostructured materials can exhibit electrochemically tunable properties due to their high surface-to-volume ratio. Based on this concept, reversible tunig of mechanical, electrical, and magnetic properties has been demonstrated recently. The present work studies the tunability of the electrical resistance of nanoporous platinum, produced by dealloying of a $Cu_{75}Pt_{25}$ alloy. In the investigated potential range, the charge coefficient $(\Delta R/R_0)/\Delta Q$ exhibits a sign inversion, thus differing from previous results on nanocrystalline, compacted platinum powder [1] as well as nanoporous gold [2]. The resistance behavior in the two charge-coefficient-regimes is attributed to variations in the charge carrier density and interfacial scattering in the positive, as well as the oxygen coverage in the negative sign region. Financial support by the FWF Austrian Science Fund is appreciated (project S10405-N16).

[1] M. Sagmeister et al., Phys. Rev. Lett. **96**, 156601 (2006)
[2] P. Wahl et al., J. Appl. Phys. **108**, 073706 (2010)

MM 17.31 Mon 17:00 Poster B

Atom probe specimen preparation from nanoporous materials — •Björn Pfeiffer, Torben Erichsen, Eike Epler, and Carsten Nowak — Georg-August-Universität Göttingen, Institut für Materialphysik

During the last years open-celled nanoporous foams attracted a lot of attention because of their physical properties and possible technical applications. For example, with their large surface to volume ratio they are ideal for application as catalysts and as electrodes in batteries. To determine the chemical composition of such heterogeneous materials in three dimensions with sub-nanometer resolution atom probe (AP) exactly fits the requirements. However, problems with mechanical stability during analysis and with data reconstruction arise when analyzing non-compact materials. Here, we demonstrate that electron-beam induced CVD is a promising approach to overcome these problems.

For the experiments, nanoporous gold (np-Au) was used as a model system for nanoporous materials. Electron beam induced CVD of organometallic precursors allows to fill the pores of the material in volumes large enough for AP sample preparation with residual voids in the low nanometer range. Fieldevaporation series in FIM with intermediate TEM-imaging reveal that controlled fieldevaporation of both, np-Au and the deposited precursor is possible and that samples are mechanically stable under electric fields necessary for FIM-imaging. The presented results give an outlook on the opportunities given by this method to analyze open-celled nanoporous materials with FIM and AP.

MM 17.32 Mon 17:00 Poster B

Structural aspects of hydride formation in Gd thin films — •Sara Wanjelik, Volkmar Hess, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Hydrogen in metals has attracted a lot of attention in the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamentel point of view.

For our research we use Gadolinium grown on a W(110) crystal. Depending on the preparation conditions smooth films or islands can be obtained. The investigations were performed with a scanning tunneling microscope. It can also be used in the spectroscopic mode. This allows us to correlate hydrogen-induced electronic and topographic changes on the atomic scale. Offering high amounts of hydrogen to Gd thin films results in the formation of hydrides which exhibit a significantly enhanced lattice volume. Thus, structural changes occur in order to reduce the stress. As a result the surface shows different types of morphological variations. These changes are studied as a function of film thickness.

MM 17.33 Mon 17:00 Poster B

Lithium Iron Phosphate as thin film cathode and in all solid-state batteries — •Mathias Köhler, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Lithium Iron Phosphate (LFP) is widely used as a cathode material in conventional lithium ion batteries. In this work, thin films of LFP, exhibiting a thickness between 200 and 500 nm, were prepared by rf-ion beam sputter deposition. The films were characterized by means of X-ray diffraction (XRD), transmission electron microscopy (TEM), cyclic voltammetry (CV), and galvanostatic intermittent titration technique (GITT). The LFP films were deposited on silicon substrates at different temperatures between 400°C and 700°C. In all cases, TEM measurements show smooth and homogeneous layers, and XRD results indicate the desired crystalline structure. For detailed electrical characterisation, an additional metallic current collector (Pt, Au) of about 100 nm was deposited, so the electrochemical functionality of the samples could be investigated. First CV results show that the deposition temperature strongly influences the electrochemical capacity, and that a temperature of around 500°C results in LFP thin films of a maximum storage capacity of about 60 mAh/g. Since the thin films reveal a well-defined thickness, they give the possibility to precisely determine the diffusion coefficient of lithium in LFP by means of GITT. So, the diffusion coefficient as a function of the lithium concentration was determined, using the GITT thin film approach.

MM 17.34 Mon 17:00 Poster B

Investigation of freeze casting at the microscopic scale — •Marcel Huber[1], Frank Wendler[2], and Britta Nestler[1,2] — [1]IAM-ZBS, Karlsruhe Institute of Technology — [2]IAM-ZBS, Karlsruhe University of Applied Science

Motivated by freeze casting, an established process to produce ceramic materials with an open pore structure, we study ice crystal growth by using a phase-field model of Allen-Cahn type. The representation of each ice-crystal of different orientation and the liquid is defined by introducing non-conserved order parameters. The solid/liquid interfaces evolve due to an interplay of a driving force and of interface anisotropies with a normal velocity depending on a chemical potential, kinetic coefficient and surface stiffness. We present an anisotropy formulation for interface energies and kinetics suitable for ice-crystallization by a combination of selected spherical harmonics. We introduce an efficient numerical method based on the definition of appropriate boundary conditions to solve the dynamics of the thermal field. We show the dendritic growth shapes and evaluate the tip velocities. We investigate the solidification of ice in a pure water-ice system where water freezes by cooling from one side (cooling plate). By changing the temperature gradient, we evaluate the velocity of the solid/liquid interfaces and compare our results with experimental observations. With regard to the freeze casting process, we analyse the freezing process in a water system filled with inert particles. In simulations, we study the interaction of the particles with the growing ice front and among each other.

MM 17.35 Mon 17:00 Poster B

Silicon nanowires as anode electrodes for lithium ion batteries — •Gibaek Lee[1,2], Stefan L Schweizer[2], and Ralf B Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials Halle — [2]Martin-Luther-University Halle-Wittenberg

It has been known for some time that silicon can incorporate large amounts of Li with a specific capacity of 4200 mAh/g, about a factor of 11 larger than for state of the art graphite anodes. However, silicon and silicon-based negative electrodes exhibit huge volume expansion (ca. 270%) during lithium insertion and extraction, resulting in mechanical disintegration of electrode and rapid capacity fading. One way to overcome the problem of large volume expansion is to design three-dimensional porous electrode structures with sufficient porosity to accommodate the volume expansion. In this study, we prepared oriented silicon nanowire arrays (SiNWs) on n-type silicon substrate by metal assisted chemical etching in aqueous HF solution containing AgNO3. In addition, to reduce the usage of thick silicon substrates and extend applications of silicon micro/nanostructures on various substrates, we have developed ways to detach these SiNWs from bulk silicon substrate because particularly, the contribution of silicon wafer substrate could not be excluded from the capacity of the anode substrate.

MM 17.36 Mon 17:00 Poster B

Surface changes of defect-rich Palladium films under hydrogen atmosphere — •Marc Waninger and Astrid Pundt — Instiute of Material physics, University of Goettingen Friedrich-Hund-Platz 1, D-37077 Goettingen, Germany.

Because of the large out-of-plane expansion of thin films during hydride formation, phase transformation can be studied by surface analyses.[1] In this paper, we artificially generate surface-defects and study their influence on hydride formation by means of atom force microscopy (AFM).

200 nm Palladium films, prepared by ion-argon-beam sputtering at room temperature, are indented by an AFM Cantilever using different loads. Thereby, indentation craters of different size and shape are generated. Subsequent surface changes during hydrogen loading are studied by performing AFM measurements in a gas loading setup.

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

[1] K. Nörthemann and A. Pundt, Phys. Rev. B 78, 014105 (2008), Phys. Rev. B 83, 155420 (2011)

MM 17.37 Mon 17:00 Poster 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-iron 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-iron 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 17.38 Mon 17:00 Poster B

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

A new cluster deposition system for the synthesis of materials composed of mass-selected clusters embedded in matrices of other materials as well as cluster-decorated surfaces was constructed. This approach can open pathways to a new class of materials with tailored electronic, magnetic or catalytic properties.

The clusters are prepared in a source that combines magnetron sputtering and gas-phase aggregation. This allows the production of clusters of various materials with sizes ranging from a few atoms up to several nm. The ionized clusters are first shaped into an ion beam, then mass selected in a 1.4 T sector magnet and finally deposited on

a substrate with deposition energies ranging from 0.1 to 100 eV/atom. This covers the whole range from soft-landing up to energetic impact conditions at which the clusters are immobilized and embedded in the substrate. The matrix material can be optionally co-deposited using a high temperature effusion cell or an electron beam evaporator. Altogether the new system is a versatile instrument to synthesize nearly every type of cluster-based materials.

MM 17.39 Mon 17:00 Poster B

Coating Nanoporous Gold by pulsed electrodeposition — •Tobias Kitzler[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Germany

Over the last two decades nanoporous metals produced by selective dealloying have attracted lots of attention. Due to their enormous surface to weight ratio they exhibit outstanding electrochemical properties with respect to their mass/volume. Recently nanoporous materials became more and more interesting for battery applications not only due to their electrochemical properties, but also due to their elastic properties, i.e. the extended elastic range which might be helpful with respect to the cycle stability of the electrodes. To make the nanoporous metal applicable for different usages, e.g. Li storage, it would be interesting to produce nanoporous metals with a coated surface. Successful attempts of such a synthesis were usually limited to very thin coatings or even monolayers.

This work is about the synthesis of nanoporous Au coated with Sn by electrodeposition. The deposition of more than a monolayer is a challenging task. This probably is caused by the low mass transfer rate into the bulk of a nanoporous sample by the electrolyte. In order to circumvent those difficulties, a pulsed electrodeposition method under a continous electrolyte flow is used. By this method, the electrolyte inside the nanoporous metal is exchanged after each pulse. The samples then were characterised by SEM and EDX and the influence of the system parameters on the electrodeposition process was investigated.

MM 17.40 Mon 17:00 Poster B

On the Interpretation of ELNES - Spectra in the $Al_{1-x}Ti_xN$-System — •Simon Lamowski, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg Institut für Theoretische Physik, Leipziger Str. 23, 09596 Freiberg, Germany

In the particular system studied here layered structures were characterized by Electron energy-Loss Near Edge Structures (ELNES) measurements scanned along a perpendicular direction with respect to the interface.

By means of ab initio Density Functional Theory (DFT) calculations using a Projected Augmented plane Wave (PAW) basis set as implemented in the Abinit code we investigate structural and electronic factors which influence the ELNES. Further , we go beyond standard DFT by solving the Bethe * Salpeter - Equation to obtain the ELNES - spectra using the YAMBO package.

MM 17.41 Mon 17:00 Poster B

Simulation of diffusion processes in Ni and Al, due to the vacancy mechanism in metals on the basis of effective medium theory — •Sergiy Zamulko, Dmitriy Kropachev, and Ganna Kholmska — National Technical University of Ukraine 'Kyiv Polytechnic Institute', Kyiv, Ukraine

In our work we calculated vacancy diffusion processes in nickel and aluminium that based on the effective medium theory. The computer modeling based on the effective medium theory and Atomic Simulation Environment software. The methodic of vacancy diffusion coefficient calculations in metals that based on the effective medium theory has been developed. The computer modeling of vacancy self-diffusion processes in nickel and aluminium has been carried out using the effective medium theory. It has been stated that self-diffusion coefficient of nickel is $0{,}58*10^{-17}$ m^2/s, selfdiffusion coefficient of aluminium is $0{,}3*10^{-12}$ m^2/s. Obtained results can be used for the further calculations of diffusion processes in metal materials on the base of the effective medium theory. And also using of effective medium theory allow accelerating the time for calculations comparing to classical DFT methods.

MM 17.42 Mon 17:00 Poster B

Interaction of Ultrashort XUV pulses with Bulk Magnesium and Copper — •Naira Grigoryan, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University Kassel, Heinrich-Plett-Str. 40, Kassel, Germany

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 [Nagler et al.]. The next step is the formation of warm dense matter. In this work we perform all-electron ab initio calculations in order to determine the main pathways from solid to warm dense magnesium and copper. Surprisingly, frozen phonon calculations for the transverse and longitudinal modes at the M point lying at the boundary of the Brillouin zone of magnesium reveal hardening as a function of the electronic temperature in the laser-excited state for LO, LA, TO(perp), TA(perp) and softening for TO(parallel), TA(parallel), and hardening for all modes, as a function of temperature, in the presence of a core-hole. For the copper TA mode at the X point we also find hardening as a function of the electronic temperature in the laser-excited state and in the presence of a core-hole, which is opposite to the behavior of most materials, which soften in at least some directions when electrons are excited.

MM 17.43 Mon 17:00 Poster B

Study of viscoelastic properties of nanoporous gold using dynamic mechanical analysis — •Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, 21502 Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, 21073 Hamburg, Germany

Nanoporous (np) metals fabricated by alloy corrosion have attracted a considerable attention due to their high specific surface area and open nanoligament structure, which can be modified chemically or electrochemically. Unlike bulk nanocrystalline materials, here one can expect not only size-dependence effects of mechanical properties but also significant influence of capillary forces on the elastic and plastic behavior. Recently, it was shown that the mechanical strength of np-Au imbibed with electrolyte can be changed by a factor of 2 by controlling the electrode potential [1]. The aim of this study is the investigation of the change of elasticity of np metals in response to potential changes. We present in-situ experiments in a dynamic mechanical analysis device equipped with an electrochemical cell. The measurements were carried out while electric potentials are applied to a np-Au sample immersed in an electrolyte. Measured storage and loss moduli as well as the damping coefficient upon changing the surface state are discussed.

1. H.J. Jin, J. Weissmüller, Science, 332, 1179 (2011).

MM 17.44 Mon 17:00 Poster B

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

Hydrogen absorption behavior was investigated by in-situ XRD for nano-crystalline Mg thin films at room temperature. Nanocrystalline Mg films with 20nm-thick Pd capping layer were prepared in an UHV chamber, by means of ion beam sputter deposition. XRD measurements using a Phillips X-Pert diffractometer with Co-K alpha radiation were performed before and after hydrogenation to check the phase transition and the change of the sample texture. Thickness changes of films before and after hydrogenation were measured by a Dektak 150 profiler in order to monitor the volume change due to the hydride formation. In-situ XRD measurements have been done at synchrotron facilities. Changes of the resistivity during hydrogenation were also monitored by four-point measurement, during hydrogen gas-loading at several pressures. Reaction kinetics of nano-crystalline Mg thin films with hydrogen at room temperature is estimated from in-situ synchrotron XRD measurements and compared with the results of in-situ electrical resistivity measurements and electrochemical hydrogen permeation measurements. Financial support by the DFG via PU131/9, HASYLAB and ESRF is gratefully acknowledged.

MM 17.45 Mon 17:00 Poster B

Combining ab initio with data mining techniques: Solution enthalpy of hydrogen in transition metals — •Ugur Aydin, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Combining ab initio calculations with data mining techniques we identify a master curve for the solution enthalpy of H in 3d transition metals and related materials. Assuming nonmagnetic fcc crystal structures we find two different classes of materials, with either the octahedral or the tetrahedral interstitial site being preferred by hydrogen. An interaction radius for H in octahedral (tetrahedral) site of ≈ 0.7 Å (≈ 0.4 Å)

turns out to be a characteristic value, for which the chemical interaction energy has an optimum for all studied elements. These trends are explained in terms of fundamental band structure parameters.

MM 17.46 Mon 17:00 Poster B

Study of field evaporation from metal tips by using a custom tunable laser-assisted field ion microscope (FIM) — •Armin Feist[1,2], Johannes Endres[1], Carsten Nowak[2], and Claus Ropers[1,2] — [1]University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for Materials Physics, 37077 Göttingen, Germany

In the recent past, field ion microscopy (FIM) and atom probe tomography (APT) have shown their potential as versatile tools for studying materials interacting with ultrashort laser pulses at an atomic scale. In order to examine the physical processes involved in laser-assisted field evaporation from nanoscale tips, a conventional FIM was equipped with a tunable femtosecond laser system. We study the evaporation by differential image analysis in FIM mode, as opposed to direct detection of evaporated sample atoms as in APT. The advantage of this approach lies in its capability to atomically resolve the surface structure during the continuous evaporation process. Wavelength, static field and fluence dependent measurements on W and Mo yield insight into the microscopic evaporation mechanism and support thermal activation, while being inconsistent with the optical rectification model.

MM 17.47 Mon 17:00 Poster B

Band structure und electronic transport properties of cobalt decorated carbon nanotubes — Jan Sommer[1], •Andreas Zienert[2], and Jörg Schuster[3] — [1]Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, 09126 Chemnitz, Germany — [3]Fraunhofer Research Institution for Electronic Nano Systems, 09126 Chemnitz, Germany

Carbon nanotubes (CNTs) are promising candidates for replacing copper wires in novel interconnect structures. For such an application, it is necessary to use metallic CNTs in order to compete against conventional copper technology. However, only one third of the CNTs grown by chemical vapor deposition are metallic. A method for turning semiconducting CNTs into metallic ones would be highly desirable [1].

As a simple approach, we modeled the effect of a few cobalt atoms, placed on the surface of a semiconducting CNT, on band structure and transport properties by using density functional theory. Even a very small amount of cobalt could significantly alter the band structure by inducing spin polarized states near the Fermi energy. Transport calculations confirm, that the conductivity of the semiconducting single-wall CNT is significantly increased. Furthermore, we present results about the geometry of the cobalt decorated CNT and the influences on band structure and transport.

[1] Kim et al. ACS Nano 3, 2818 (2009)

MM 17.48 Mon 17:00 Poster B

nanoscale solid-solid dissolution of crystalline/amorphours nanoparticles by electron beam irradiation — •Tao Feng[1,2], Di Wang[1], Ralf Witte[1], Robort Kruk[1], Horst Hahn[1], and Herbert Gleiter[1] — [1]Karlsruhe Institute of Technology, Institute for Nanotechnology, Karlsruhe, Germany — [2]Engineering Research Center for Nanophotonics & Advanced Inst6rument, Ministry of Education, Department of Physics, East China Normal University, Shanghai, China

The diffusion behavior between different chemical composition nanoparticles is very critical for understanding the performance stability and lifetime of nanoparticles. Here, we report a systematic study carried out "in-situ" in the transmission electron microscopy (TEM) on an electron-irradiation-induced transformation of crystalline Pd/amorphous $Fe_{25}Sc_{75}$ core/shell nanoparticles, which are prepared by co-evaporation Pd metal and $Fe_{45}Sc_{55}$ alloy in an inert gas condensation (IGC) system. Under the low electron beam irradiation (below 1×10^6 electrons $nm^{-2}s^{-1}$), the crystal lattice of Pd disappeared gradually, accompanying with the growth of Pd domain. High-sensitivity energy-dispersive X-ray (EDX) spectroscopy give the direct evidences of the atomic diffusion between Pd and Sc, which cause to form an new amorphous compound of PdFeSc in the core/shell nanoparticles. Such physical manipulations of nanoparticles can be exploited as a tool to access novel nanoglass.

MM 17.49 Mon 17:00 Poster B

Compositional changes during phase separation of $\gamma\prime$ precipitates in a Ni-Al-Ti model alloy — •Florian Vogel, Nelia Wanderka, and John Banhart — Helmholtz Zentrum Berlin GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The phase-separation phenomenon of $\gamma\prime$ precipitates in a single crystal Ni-8.5Al-5.4Ti (at.%) model alloy was investigated by means of transmission electron microscopy (TEM) and three-dimensional atom probe (3D-AP). After homogenization, ageing at 1213 K led to formation of the initial $\gamma/\gamma\prime$ microstructure composed of cuboidal $\gamma\prime$ precipitates embedded in a γ matrix. Subsequent ageing at 1023 K resulted in the formation of new particles within the $\gamma\prime$ precipitates. Ex-situ TEM was used to follow the influence of these particles on the evolution of microstructure and the kinetics of $\gamma\prime$ coarsening. 3D-AP revealed the chemical composition of the γ matrix, the $\gamma\prime$ precipitates and the particles within $\gamma\prime$. It was found that the particles are rich in Ni and poor in Ti as compared to the $\gamma\prime$ precipitates. The results are discussed with respect to the solubility of Ni within the $\gamma\prime$ phase based on heat treatment conditions.

MM 17.50 Mon 17:00 Poster B

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. Comparisons of volume expansion coefficients and C_p-values with experiment for the wurtzite phase show the accuracy of the method.

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

MM 17.51 Mon 17:00 Poster B

Influence of Quenching & Partitioning on martensite and austenite phase composition in steel — •Karin Rüster[1], Andre Steffen[1], Michael Paulus[1], Christian Sternemann[1], Metin Tolan[1], Niko Grosse-Heilmann[2], Christian Kronholz[2], and Andreas Peters[2] — [1]Fakultät Physik / Delta, TU Dortmund, Germany — [2]Benteler Tube Management GmbH, Paderborn, Germany

Steel is a common material in our daily life. Macroscopic characteristics (e.g. hardness, tensile properties...) of steel are affected by the crystalline structure, i.e. austenite and martensite phase, which is changed during heat treatment. During the process of Quenching and Partitioning carbon diffuses from martensite to austenite, enriches the austenite and thereby stabilises the phase of austenite. This way a microstructure with retained austenite is produced. To analyse the influence of heating and cooling XRD-experiments have been carried out, ex-situ for pre-treated samples and in-situ. The experiment was performed at beamline BL9 at Delta.

MM 17.52 Mon 17:00 Poster B

Microstructure of InAs nano-crystals embedded in Si — •Mingjian Wu[1], Achim Trampert[1], Tariq Al-Zoubi[2], Muhammad Usman[2], Mohamed Benyoucef[2], and Johann Peter Reithmaier[2] — [1]Paul-Drude-Institut für Festköperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Institute of Nanostructure Technologies and Analytics, CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany

In this work, the structural properties of InAs nano-crystals embedded in a Si matrix are investigated by transmission electron microscopy (TEM). The InAs is grown on Si (001) by molecular beam epitaxy at 400 °C and subsequently overgrown by Si at 700 °C. Depending on the nominally deposited amount of InAs, the embedded clusters show spherical and truncated octahedral-like shapes with {111} and {001} facets, which are significantly different to the initially flat InAs islands. The bulk lattice mismatch of 10.4 % is relieved by dislocation loops along the interface consisting of perfect 60°-type dislocations and partial dislocation with stacking faults inside the InAs clusters.

By two-dimensional strain mapping derived from high-resolution TEM structure images, no strain gradients in the Si matrix around InAs clusters are detectable. On the other hand, anisotropic lattice distortions inside the InAs clusters are identified, which are characterized by compressive and tensile strain distributions in the two mapped directions, i.e. parallel and perpendicular to the growth direction. This residual strain is discussed based on the thermal mismatch between InAs and Si.

MM 17.53 Mon 17:00 Poster B

Is the epsilon-phase in deformed autenitic steel just an accumulation of stacking faults? — •Torsten Weissbach, Sebastian Schwalbe, Jürgen Kutzner, and Jens Kortus — Institut f. Theoretische Physik, TU BergAK Freiberg, 09596 Freiberg

Highly alloyed TRIP steels consisting of metastable austenite show a transformation induced by deformation to the hexagonal lattice known from the hcp phase of iron. It has been shown by other authors that the X-ray data proving this can also be interpreted as stacking faults, because they usually occur on hexagonal planes in cubic Fe. Furthermore, the stacking fault energy in TRIP steel is low compared to other steel types.

We show density functional theory calculations on Fe to address the question under which conditions the hcp phase can be stable. Because the alloyed steel exhibits considerably strained lattice parameters, we are particularly interested in the behaviour of Fe under such conditions. The Fe phases are a complicated system for DFT; calculations are known to be very sensible to the type of exchange-correlation functional.

MM 17.54 Mon 17:00 Poster B

Gas diffusion electrode development using femtosecond-laser induced microstructured metal surfaces with hydrophobic features — Andreas Gabler[1], Anna-Lena Baumann[1], Thomas Gimpel[2], Stefan Kontermann[1], Robert Hahn[3], and •Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, 38640 Goslar — [2]Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — [3]Fraunhofer Institute for Reliability and Microintegration, IZM, 13355 Berlin

At present, hydrophobic characteristics of gas diffusion electrodes are mostly generated by using polytetrafluoroethylene-materials (PTFE).

An innovative, methodic approach of directly generating new hydrophobic metal surfaces is developed by using femtosecond-laser induced microstructures through ablation, similar to the so called Black Silicon Material.

Its characteristic appearance is a spike-structure at micrometer level, in which superhydrophobic characteristics have already been successfully achieved. Preliminary analyses examined the good usability of the fs-laserprocess in cases of surface structuring on different metals.

The direct generation of microstructured metal surfaces with hydrophobic characteristics for gas diffusion electrodes has the advantage of being a one-material-system with the combined features of hydrophobicity, electrical conductivity und large catalyst surface at a three phase boundary .

In this case, different process settings were made and the resulting surface structures and hydrophobic characteristics compared.

MM 17.55 Mon 17:00 Poster B

In-situ observation of structural changes accompanying lithium intercalation in silicon TEM lamellas — •Timo Wuttke, Burkhard Roos, Carsten Nowak, and Cynthia Volkert — Georg-August-Universität Göttingen, Institut für Materialphysik

In-situ studies of electrochemically driven lithiation and delithiation of materials for lithium-ion-batteries promise an improved understanding of the underlying intercalation mechanisms. We report the construction of a miniature lithium-ion-battery inside a transmission electron microscope using a STM-TEM holder. The cathode consists of a $LiMn_2O_4$-particle, while a silicon TEM lamella is used as anode. A liquid electrolyte ensures a high ionic conductivity between both components. It is based on an organic conducting salt dissolved in an organic ionic liquid and has a very small vapor pressure, enabling its use in the high vacuum of a TEM.

Crystalline silicon experiences several phase transitions with increasing amount of lithium and is amorphous once fully lithiated. Structural changes of both cathode and anode during lithiation are studied. Current-voltage characteristics, volume expansion and amorphization during lithiation are discussed.

MM 17.56 Mon 17:00 Poster B

Lithium ion dynamics in channel-structured $Li_2Ti_6O_{13}$ — •Kai Volgmann and Paul Heitjans — Leibniz Universität Hannover, Inst. f. Phys. Chemie u. Elektrochemie, Callinstraße 3 - 3a, D-30167 Hannover

Solid-state nuclear magnetic resonance (NMR) spectroscopy subsumes a couple of powerful techniques to investigate the diffusion of Li ions on the microscopic scale. These methods can be used, e. g., to investigate effects on the motion of Li^+ ions by dimensionality reduction. In this work, $Li_2Ti_6O_{13}$ (space group C m/2) has been chosen as model system due to its channel-like crystal structure. Lithium is supposed to be solely located inside the channels. Samples with varying Li content have been studied. Synthesis is done via a solid-state reaction and subsequent ion exchange of sodium ions. The samples were characterized by powder x-ray diffraction and inductively coupled plasma optical emission spectroscopy. ^{7}Li NMR relaxometry measurements have been performed at different Lamor frequencies ω_0. Due to the channel-like structure, a confined Li diffusion process is expected leading to a frequency-dependent spin-lattice relaxation rate in the regime $\omega_0 \cdot \tau \ll 1$ where τ is the motional correlation time. A blocking effect in the structure due to the sodium cations is observed for samples with substoichiometric Li concentration.

MM 17.57 Mon 17:00 Poster B

Molecular Dynamics Simulation of Aluminum Oxidation via Reactive Force Field — •Manana Koberidze and Risto Nieminen — Aalto University, School of Science, Espoo, Finland

Tunneling current in aluminium-oxide thin film based nano-electronic devices is strongly dependent on the geometry of a metal-oxide interface [1], affecting the quality of the barrier, consequently, performance of a device. Therefore, it is crucial to know the structure of the interface and kinetics of its formation. Most of the works addressing aluminum oxidation consider only initial stages at low coverage. Rather little information is available about the interfaces in question.

Our goal is to achieve detailed understanding of oxide growth via molecular dynamics simulations, further, to develop quantitative description of transport relevant barriers. We use Reactive Force Field (ReaxFF) [2] which has been successfully exploited for Al/Al_2O_3 interface and is claimed to be fully transferable for the description of oxidation process [3]. Simulated results for Al(111) oxidation above one monolayer coverage will be presented. Calculations are performed in the near-room-temperature range, thereby assessing the applicability of ReaxFF to the current problem.

References:
[1] V.F. Maisi, et al., PRL 106 (2011) 217003.
[2] A.C.T. van Duin, et al., J. Phys. Chem. A 105 (2001) 9396.
[3] Q. Zhang, et al., Phys. Rev. B 69 (2004) 045423.

MM 17.58 Mon 17:00 Poster B

An approach for quantitative assessment of shear induced mixing in mechanical alloying — •Mohsen Pouryazdan[1], Di Wang[1], Torsten Scherer[1], Robert Averback[2], and Horst Hahn[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021, Karlsruhe, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, 1304 W. Green St., Urbana, IL 61801, USA

A critical feature in the processing of nanocomposites is the forced mixing of alloying components. By forced mixing we refer to the atomic mixing of atoms attributed to shear deformation. Presently, this process is only poorly understood. This lack of understanding is partly because nearly all of our information to date has been derived from experiments employing ball milling (BM), for which the mixing conditions: strain rate, total strain, temperature, and stress state are poorly characterized. In contrast to experiments using BM, our experimental approach using high pressure torsion (HPT) allows quantitative assessment of mixing conditions. In the current study, Ag60Cu40 two-phase immiscible alloy was processed by HPT for various levels of strain. The state of intermixing was investigated by XRD, DSC and TEM.

It is observed that the rate of chemical disordering increases with the accumulation of applied strain. A complete chemical homogenization of the original lamellar structure of Ag60Cu40, with periodicity of ~165 nm, is achieved after a shear strain of ~725 at a shear strain rate of ~1.5 1/s. The chemical mixing is accompanied by extensive grain refinement leading to nanocrystalline grains with average size of ~42 nm.

MM 17.59 Mon 17:00 Poster B

Origin of high Neel temperatures in Tc perovskites — Jernej Mravlje[1,2,3], Markus Aichhorn[4], and •Antoine Georges[1,2] — [1]College de France, Paris, France — [2]Ecole Polytechnique, Palaiseau, France — [3]Josef Stefan Institue, Ljubljana, Slovenija — [4]TU Graz, Austria

Very recently, antiferromagnetism persisting to high temperatures exceeding 1000K was discovered in Tc perovskites. Usually, robust magnetism is associated to 3d transition metal oxides, moreover in 4d oxides magnetism is rarely found. Here we describe results of LDA+DMFT calculation of electronic structure of two cubic perovskites, SrMnO3 and SrTcO3. The Neel temperature of SrTcO3 is found 4 times larger, in agreement with experiment. Smaller Tc moment is reproduced aswell. We show that the distinction between the two materials is that Tc is far more on the itinerant side, and found in the immediate proximity to the metal-insulator transition in the paramagnetic state. Accordingly, the dependence of Neel temperature on pressure is very weak in strong violation of the Bloch's law.

MM 17.60 Mon 17:00 Poster B

Hybrid material design with DFT: Silane coupling agent on TiO_2(011) — •Wolfgang Heckel, Beatrix Elsner, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

In order to control the mechanical properties of hybrid materials, the detailed knowledge of the interfaces, the atomic structure and stability is crucial. Density functional theory (DFT) allows for the investigation of the local electronic structure and the determination of desired observables like binding energy.

Using the TiO_2 bulk rutile structure as a starting point, we develop a model system for the interface between the adsorbing silane coupling agents and the TiO_2(011) surface representing a ceramic-polymer junction. Here, a good choice for the exchange-correlation functional plays an essential role. We find that the release of bonding energy depends heavily on the adsorption sites and the energetically most favourable molecular arrangements show only weak bonding to the surface. The tendency of the adsorbing molecules to form clusters before adsorption will be discussed.

MM 17.61 Mon 17:00 Poster B

Simulation of structural phase transitions and shape memory behavior in NiTi nanosystems — •Daniel Mutter and Peter Nielaba — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

We present results of atomistic molecular dynamics simulations of structural phase transitions and shape memory behavior of NiTi nanosystems. The application of heating-cooling cycles to bulk systems (2000 atoms under periodic boundary conditions) confirmed the experimentally known strong dependence of B19'-to-B2 transition temperatures (TTs) on alloy composition, which could be related to an increasing lattice instability, arising when the perfect ordered composition with 50% Ni and 50% Ti is changed slightly [1]. By applying free boundary conditions, spherical NiTi nanoparticles are simulated, showing a size dependence of the TTs. Further calculations suggest this to be due to an increasing surface-to-volume fraction and therefore a major influence of the surface free energy when the system size is reduced [2]. In addition, the nanoparticles show twinning of differently orientated variants of a B19'-like structure at low temperatures. We apply loading-heating-cooling cycles to these systems, which shows a shape memory behavior at the nanoscale differing from the known bulk mechanism.

[1] D. Mutter and P. Nielaba, Phys. Rev. B 82, 224201 (2010).
[2] D. Mutter and P. Nielaba, Eur. Phys. J. B 84, 109 (2011).

MM 17.62 Mon 17:00 Poster B

Modeling the crystal growth phenomena on atomistic scale in single crystals and binary alloys — •Muhammad Ajmal Choudhary[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Institut für physics, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

The phase field crystal (PFC) technique is a novel approach for modeling crystal growth phenomena with atomistic resolution. Here we demonstrate the derivation of an anisotropic phase-field crystal (APFC) model, recently elaborated and investigated by M A Choudhary et al. [J. Phys.: Condens. Matter 23, 265005 (2011)] from microscopic density functional theory for anisotropic particles. We explored its crystal morphologies to demonstrate the influence of anisotropy and undercooling on nucleation and microstructure formation process. These stable phases are also investigated with respect to their characteristic morphological features. To describe the equilibrium properties of eutectic binary alloys in two dimensions, we develop a simple binary PFC model based on Elder et al. [Phy. Rev. B 75, 064107 (2007)]. We implement it as a real space dynamic code in two dimension. We analyze properties of metastable nuclei in the liquid-solid co-existence region and just below the eutectic point using the technique of finite system size phase transitions [Phy. Rev. E 79, 061104 (2009)]. Of particular interest is the growth of a secondary solid phase on a primary nucleus occurring during eutectic solidification.

MM 17.63 Mon 17:00 Poster B

Simple Synthesis of Metal and Metal Oxide Nanowires for Device Application — •Pervin Sahin, Necdet Onur Urs, Dawit Gedamu, Torge Behrendt, and Rainer Adelung — Functional Nanomaterials, Institute for Material Science, Faculty of Engineering, University of Kiel, Germany

1-dimensional metal and semiconductor nanostructures exhibit interesting physical properties but their integration into modern electronic devices is often a very challenging task. Finding the appropriate supports for nanostructures and nanoscale contacts are highly desired aspects in this regard. In present work we demonstrate the fabrication of 1D nano- and mesostructures between microstructured contacts formed directly on a silicon chip either by a thin film fracture (TFF)[1] approach or a delamination approach. Both approaches offer the possibilities to integrate the obtained nano- meso structures in wafer level fabrication. Recently, a novel approach named hot plate delamination approach allowed to fabricate connected single crystalline iron oxide nanowires from delaminated and microstructured iron films in a self organized way on a hot plate. Electrical properties of these nano-micro structures integrated on Si-chips and their preliminary applications towards sensors and field effect transistors are presented as well.

[1]Dawit Gedamu, Ingo Paulowicz, Seid Jebril, Yogendra Mishra, and R. Adelung, Journal of Nano Technology, October 2011(in press)

MM 17.64 Mon 17:00 Poster B

Exploring GPUs for Mesoscale Simulations — •Alexander Monas, Claas Hüter, and Robert Spatschek — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The modeling of microstructure evolution like solidification or solid state transformations as well as many other pattern formation processes in general requires the solution of coupled partial differential equations. This is in particular the case for phase field modeling, where the motion of phase fronts is represented by the temporal evolution of an order parameter field. These simulations are very time consuming, and therefore frequently massive parallelization is used to accelerate the computations. Here we report on implementations on (consumer) graphics cards, which have a theoretical peak performance of more than 1 TFlop. We demonstrate the efficiency of this approach for diffusion problems and phase transformation processes, where we use real space implementations in two and three dimensions. For amplitude equation models, which are derived from classical density functional theory, we use pseudospectral methods. The efficiency of the GPU implementations is shown for solid-liquid interface interaction and for dislocation pairing transitions at hot grain boundaries.

MM 17.65 Mon 17:00 Poster B

Hydrogenation of Magnesium Titanium Multi- Layers — •Jara Kürschner, Helmut Uchida, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Freidrich-Hund-Platz 1, 37077 Göttingen

Magnesium is a promising metal for hydrogen storage as it can store up to 7.6 weight% H. But, its hydrogen sorption kinetics are very slow. Magnesium can be combined with metals such as titanium, which have fast hydrogen sorption kinetics and do not alloy in equilibrium.

In this work, the hydrogen absorption properties of different magnesium titanium multi-layer stacks are investigated by electrochemical loading at room temperature. The palladium-capped samples are prepared by ion beam deposition on cleaned substrates and structurally analysed by X-ray diffraction.

Their properties such as hydrogen pressure and transmittance are analysed in dependance of the connection to the substrate and the Pd cap, the layer stacking, and the layer thickness.

This research is kindly supported by DFG PU131/9.

MM 17.66 Mon 17:00 Poster B

Interfaces in Fe/MgO/Fe sandwich structures — •Torben Boll[1], Talaat Al-Kassab[1], Catharina Wille[1], and Ryota Gemma[2] — [1]King Abdullah University of Science & Technology, Division of Physical Sciences, Thuwal, Kingdom of Saudi Arabia — [2]Institut für Materialphysik, Göttingen, Germany

Electronic devices, based on the Tunnel Magneto-Resistance (TMR) effect, which are consisting of multi layered structures, are of emerging interest. The magnetic properties of such multilayer structures are governed by the properties of the metal/oxide interfaces. This paper focuses on Atom Probe Tomography (APT) investigations of the interfaces in such multilayer structures.

Fe/MgO/Fe/Au layer structures were deposited on Si-microtips by Ar-sputtering. The Au-layer is meant to prevent oxidation when the sample is exposed to the air. Results of different thermal treatments will be presented in this study to elaborate the mixing effects at the metal/oxide interface. The APT measurements were performed with the LEAP 4000 HR at the King Abdullah University of Science & Technology.

MM 17.67 Mon 17:00 Poster B

Analysis of the nitrogen content of carbide particles in a gamma'-strengthened Ni-based superalloy — •Martin Peterlechner, Harald Rösner, and Eckhard Nembach — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm Klemm Straße 10, 48149 Münster, Germany

Ni-based superalloys are commercial construction materials used at elevated operating temperatures. Carbide particles contribute to their mechanical properties. In the past these carbides were referred to as carbo nitrides but it is a question of long standing whether they do contain nitrogen and if so in what concentration. We have examined the nitrogen content of carbide particles of (Ti,Mo)-C carbides in a commercial superalloy (NIMONIC PE16) by electron energy loss spectroscopy (EELS) and energy dispersive X-ray analysis (EDX). The results suggest that the content of nitrogen in these carbides is negligible.

MM 17.68 Mon 17:00 Poster B

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

The oscillation behaviour of Silicon nanomechanical resonators in the form of doubly clamped beams is investigated by Molecular Dynamics simulations using the Stillinger-Weber interaction potential. After setting up the initial structure using a diamond lattice and a (2×1) symmetric dimer surface reconstruction, the end points of the beams are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the beams. Besides varying the size of the beams, the effects of temperature and external stretching fields are explored. The results show a decrease of the oscillation frequencies with rising temperature and a strong increase of the damping coefficient, a strong increase of the frequencies with external stress (stretching) and a decrease of frequencies with length. Other materials (e.g. NiTi memory alloys) are explored as well.

MM 17.69 Mon 17:00 Poster B

Hydrogenation behavior of thin epitaxial Nb films: Film preparation and hydrogen gas loading — •Vladimir Burlaka[1], Stefan Wagner[1], Anthony Bell[2], and Astrid Pundt[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]HASYLAB Hamburg, Germany

For thin films below a critical film thickness it was reported [1,2] that stress release via the formation of dislocations during hydrogen loading is energetically suppressed. To study this, Nb-H thin films are used as a model system. As a first step, the proper substrate temperatures for atomically smooth and epitaxial Nb film growth of thin films (20nm) on sapphire substrates during UHV sputter deposition were determined. In order to monitor hydride precipitation in the Nb films during hydrogen gas loading, in-situ STM measurements for 20 nm film thickness were performed, characterizing the films surface morphology in the as prepared and in the hydrogenated state.

Hydrogen induced lattice parameter changes of the Nb films were investigated by in-situ X-ray diffraction measurements during hydrogen gas loading at the synchrotron radiation facility in HASYLAB, Hamburg. It was shown that for a film with 20 nm, peak shifts change. We interpret this with a reduced dislocation formation.

[1] K. Nörthemann, A. Pundt, PHYS. REV. B 78, 014105 (2008)

[2] S. Wagner, H. Uchida, V. Burlaka et al., Scripta Materialia, Vol.64, Issue 10, p. 978-981 (2011)

This research was kindly supported by the DFG via PU131/9-1 and HASYLAB via project II-20060117.

MM 17.70 Mon 17:00 Poster B

Atomic scale simulations of elastic properties of Al_2O_3–C refractories — •Yuriy Natanzon and Heike Emmerich — Lehrstuhl für Material- und Processsimulation, Universität Bayreuth, Nürnberger Str. 38, 95448 Bayreuth, Germany

Aluminium oxide has a lot of significant industrial applications, in particular Al_2O_3 with 4% carbon addition is used as a refractory material. In this respect the influence of nano-additives on the elastic properties of this material is crucial to understand the phenomenon of crack propagation and fracture on atomic level. In addition, atomic scale calculations can be used as a starting point for studying this phenomenon on the macroscale. In particular, calculated elastic constants are further used for the phase field simulations of the crack propagation in ceramic refractories.

Here we present the results of molecular dynamics simulations of the dynamics of crack propagation in carbon doped α–Al_2O_3 refractories. As such simulations are time consuming, we obtain the relaxed crystal structure by means of classical molecular dynamics, and then materials properties are calculated by the combination of density functional theory and molecular dynamics. The dependence of elastic properties on both temperature and carbon content is analyzed. Our results contribute to the understanding the mechanism of bond breaking and dynamics of crack propagation on the atomic level for the purpose of designing a new fire-proof materials with reduced carbon content.

MM 17.71 Mon 17:00 Poster B

Comparison of MOKE- and SQUID-detected magnetization of FePt-layers on MgO-substrates — •Peter Jerabek[1], Thomas Bublat[2], Dagmar Goll[3], Stefan Topolovec[4], Roland Würschum[4], and Heinz Krenn[1] — [1]Karl-Franzens-University Graz, Graz, Austria — [2]Max Planck Institut für Intelligente Systeme, Stuttgart, Germany — [3]Aalen University, Materials Research Institute, Aalen, Germany — [4]Institut für Materialphysik, TU Graz, Graz, Austria

Chemically ordered FePt in the L10 phase is known as hard magnetic material with an extremely high magnetic anisotropy. From SQUID measurements [1] different mechanisms of magnetization reversal have been recognized: nucleation or pinning of domain walls depending on the layer thickness, on the degree of chemical order and on the grain size distribution. Coherent rotation or domain wiping determines the coercivity. SQUID magnetometry allows to monitor (and calibrate) the in-field- and the the out-of-field magnetization, but the Magnetooptic Kerr Effect (MOKE) provides additional information about the dynamics of magnetization reversal. The enhanced surface sensitivity of MOKE is utilized to account for the electric tunability [2] of magnetization by soaking FePt/MgO-films in KCl electrolyte, for which a special electrochemical cell including a reference electrode is designed.

[1] T. Bublat, D. Goll, J. Appl. Phys. 108 (2010) 113910

[2] M. Weisheit et al., Science 315 (2007) 349

MM 17.72 Mon 17:00 Poster B

Ehrenfest molecular dynamics within the projector augmented-wave method — •Ari Ojanperä[1], Ville Havu[1], Lauri Lehtovaara[2], Arkady Krasheninnikov[1,3], and Martti Puska[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]LPMCN, Université Claude Bernard Lyon 1, France — [3]Materials Physics Division, University of Helsinki, Finland

Modeling nonadiabatic processes, such as ion-atom collisions and electron transfer in molecular and biological systems, represents major computational challenges because multiple potential energy surfaces (PESs) are involved in the dynamics. Consequently, traditional ab initio molecular dynamics (AIMD) methods, founded on the assumption that the electronic subsystem is in its ground state, cannot be used. Ehrenfest molecular dynamics (Ehrenfest MD) within time-dependent density functional theory (TDDFT) offers a computationally affordable approach to simulating nonadiabatic processes by coupling the quantum equations of motion for electrons with classical equations of motion for nuclei via an average potential surface.

We have implemented Ehrenfest MD within the projector augmented wave (PAW) method. The electronic structure program used for the implementation is GPAW, which uses real space grids and finite differences. We demonstrate the applicability of our method by studying electronic stopping in graphene. We find that our PAW-based Ehrenfest MD results agree well with previous Troullier-Martins pseudopotential calculations. Moreover, the agreement with experiments is good as long as the effect of core electron excitations is small.

MM 17.73 Mon 17:00 Poster B

Real structure characterization of shockwave-synthesized γ-$Si_3(O,N)_4$ — •Anke Köhler[1], Christian Schimpf[2], Thomas Schlothauer[3], Volker Klemm[2], Marcus Schwarz[1], Gerhard Heide[3], David Rafaja[2], and Edwin Kroke[1] — [1]Institute of Inorganic Chemistry, TU Bergakademie Freiberg, Leipziger Str. 29, 09596 Freiberg — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Str. 5, 09596 Freiberg — [3]Institute of Mineralogy, TU Bergakademie Freiberg, Brennhausgasse 14, 09596 Freiberg

The spinel-type Si_3N_4 is known since 1999 and is counted among the hardest materials. It can be synthesized under high pressure only. Although the thermodynamic phase boundary is ~ 12 GPa, usually large overpressures are required for shock wave synthesis of larger amounts of the material. The application of amorphous precursors and peak shock pressures ≥ 35 GPa enabled us to manufacture spinel-type material in the system Si-O-N without impurities of the low pressure modifications.

The global chemical composition of the synthesized samples was investigated by means of elementary analysis (EA) and SEM/EDX. The sample with the most perfect microstructure data obtained by X-Ray diffraction shows the lowest oxygen content. Detailed microstructure analyses of the $Si_3(O,N)_4$-nanopowder using high resolution TEM confirmed the expected spinel structure. However, they disclosed some extended crystal structure defects. EELS measurements showed much broader variation of the [O]/[N] ratios than expected.

MM 17.74 Mon 17:00 Poster B

Characterization Strategies for Material Processing with Structured fs-Laser Pulses — •Conrad Schuster, Anna Svanidze, Neeke Rothe, Steffen Fiedler, Robert Irsig, Anna Oniszczuk, Josef Tiggesbäumker, Karl-Heinz Meiwes-Broer, and Stefan Lochbrunner — Institute of Physics, University of Rostock, Germany

Material processing with ultrashort laser pulses attracts considerable attention since it allows for micro machining with highest precision. The characteristics of both laser pulse and processed material determine plasma formation and the appearance of the subsequent breakdown of the material. To optimize the machining process and to understand the laser material interaction, online characterization methods are highly desirable. For this purpose we have developed two setups, one is to observe the time dependent material response on the laser pulse impact and the other is to characterize the obtained structures at the location of processing. In the first setup the output of a Ti:Sa fs laser system is split into two beams. The first beam passes through a pulse shaper and provides structured NIR pulses for the machining process. The second one is frequency doubled and the resulting blue probe pulses are guided via a delay stage through the same focusing objective as the machining pulses. The transmitted blue light is recorded by a CCD camera to study the evolution of the plasma generated by the NIR pulses. In the second setup the objective for machining is simultaneously used as the front end of a confocal microscope. This enables an online characterization of the generated microscopic structures.

MM 17.75 Mon 17:00 Poster B

NanoSculpt: a tool for generating arbitrarily shaped structures for atomistic simulations — •Martin Hummel[1], Siegfried Schmauder[1], and Erik Bitzek[2] — [1]IMWF, Universität Stuttgart — [2]Dept. Werkstoffwissenschaften, WW1, Universität Erlangen-Nürnberg

Atomistic simulation methods are becoming increasingly popular in the study of mechanical properties of materials. In particular in combination with in-situ experiments they allow the identification and detailed study of deformation mechanism. However, replicating experimentally studied specimens on the atomic scale still is an almost artisanal process. Commonly used approaches include the use of cutting planes or analytical mathematical expressions to generate geometrical shapes, or, in case of polycrystals, the use of Voronoi tessellation. Simulations using such simplified structures are very successful in providing generic information, however the specific deformation mechanisms of particular structures may depend sensitively on theire complex shape. Here we present an open-source software tool to generate complex 3D shapes for the use in atomistic simulations directly from experimental or simulation data. The tool is based on the ray-crossing algorithm from computational geometry to determine whether a given point lies inside a polyhedron. It requires triangulated surface meshes, which are commonly generated by serial sectioning or tomography methods, or can be extracted from grain growth or phase field simulations. Presented examples include grains reconstructed from serial sectioning and experiments, precipitates, nano-foams, and surface structures.

MM 17.76 Mon 17:00 Poster B

Accelerating DFT and TDDFT Electronic Structure Calculations Using Graphics Processing Units — •Samuli Hakala[1], Ville Havu[1], Jussi Enkovaara[2], Martti Puska[1], and Risto Nieminen[1] — [1]Department of Applied Physics, School of Science, Aalto University, Espoo, Finland — [2]CSC - IT Center for Science Ltd., Espoo, Finland

A Modern Graphics Processing Unit (GPU) is an efficient many-core stream processor suitable for throughput-orientated General Purpose (GP) parallel computations. Usage of GPGPU in scientific calculations has increased a lot in recent years. We have accelerated an electronic simulations software GPAW using GPUs. GPAW is a Density Functional Theory (DFT) program package based on the Projector Augmented Wave (PAW) method. Time-Dependent Density Functional Theory (TDDFT) is implemented in the linear response and time propagations schemes. Physical quantities are represented in a uniform 3D real space grid.

We have implemented GPU accelerated versions of the most numerically intensive parts in GPAW calculations using NVIDIA CUDA. Multiple GPUs and cluster nodes can be utilized with MPI using domain decomposition or by parallelizing over k-points. High performance is achieved by hand tuning the CUDA kernels and by minimizing data transfers between the GPU and the host computer. We describe our implementation and analyze the performance and the scalability of the code. Our results show that GPUs can provide significant speed-ups in both DFT and TDDFT calculations.

MM 17.77 Mon 17:00 Poster B

Enhanced Ferromagnetism in Nanometallic Glass studied by Mössbauer spectroscopy — •Ralf Witte[1,2], Tao Feng[1], Mohammad Ghafari[1], Robert Kruk[1], Richard Brand[1], Herbert Gleiter[1], and Horst Hahn[1,2] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie, D-76344 Eggenstein- Leopoldshafen — [2]Technische Universität Darmstadt, Gemeinschaftslabor Nanomaterialien, Petersenstr. 23, D-64287 Darmstadt

Interface or grain boundary effects in materials have been widely investigated since the discovery of nanocrystalline materials. In the next step these studies have been extended to another interesting class of materials such as nanoglasses or nanostructured amorphous solids. These materials can be produced by synthesis of amorphous nanoparticles in an inert-gas-condensation (IGC) process and subsequent compaction in UHV. The resulting solid material is characterised by its increased density of structural defects (interfaces) and drastically increased free atomic volume in the interfaces between the glassy nanoparticles. We report on a study using Mössbauer spectroscopy and magnetic property measurements of a nanoglass prepared from amorphous $Fe_{90}Sc_{10}$ nanoparticles. The material investigated exhibits dramatic changes in magnetic properties, namely an increased magnetic transition temperature by more than 200 K and enhanced magnetic hyperfine fields compared to the structurally homogeneous amorphous material. We attribute this newly identified magnetic phase to the glass-glass interfaces, where the decreased atomic density leads to enhanced exchange interactions following the Bethe-Slater formalism.

MM 17.78 Mon 17:00 Poster B

Kinetic processes in copper bi- and tricrystals — •Isabelle Binkowski[1], Henning Edelhoff[1], Jörn Leuthold[1], Matthias Wegner[1], Martin Peterlechner[1], Shashank Shekhar[2], Alexander King[3], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]Indian Institute of Technology Kanpur Kalyanpur, Kanpur - 208 016 — [3]The Ames Laboratory, 311 TASF, Iowa State University Ames, IA 50011-3020

Grain boundaries (GBs) and their junctions often define properties of polycrystals and have an influence on diffusion and plastic behavior.

Because of the high density of GBs included in polycrystalline materials and especially nanocrystalline materials, investigation of kinetic processes in this type of defect are of fundamental interest. Heading towards nanostructured materials one has to focus also on triple junctions (TJs) since their volume fraction and correlative their influence on materials' properties rise. In the present investigation, a near special $\Sigma(5):\Sigma(5):\Sigma(25)$ copper tricrystal is utilized to examine the properties of a TJ with defined orientation of grains and misorientation across the GBs. The mass transport properties of the tricrystal are investigated using the radiotracer method. The kinetics of out-diffusion from the TJ into the neighboring GBs are measured by preparing proper bicrystalline samples. Additionally, tensile tests including plastic deformation of several percent are performed and the digital image correlation technique is applied to measure the strain fields in the immediate vicinity of GBs and TJs.

MM 17.79 Mon 17:00 Poster B

Reactive Diffusion and Stress in Core-Shell Nanostructures — Zoltan Erdelyi[1], Christian Buchholz[2], and •Guido Schmitz[2] — [1]Department of Solid State Physics, University of Debrecen, Hungary — [2]Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

In comparison to planar multilayers, core-shell and hollow nanospheres show remarkably different kinetics of solid state reaction, since much higher levels of reaction-induced stress can develop in closed spherical geometries. We present a completely analytical model to calculate the development and anisotropic plastic relaxation of stress during reactive diffusion in spherical geometry. The complex model can be considered as a generalization of Stephenson's model (Acta Metallurgica 1988; 36:2663). It is demonstrated that growth rates in nanometric spherical diffusion couples may switch from fast Darken interdiffusion to slow Nernst-Planck interdiffusion regime in dependence of layer stacking sequence. In triple layers A/B/A, the reaction rate at both interfaces may become remarkably different as has been indeed observed experimentally (Schmitz et al. Acta Mat. 2009; 57:2673) by atom probe tomography.

MM 17.80 Mon 17:00 Poster B

Study of the EFGs at both M- and A-sites in Zr_2InC and Hf_2InC using γ-γ angular correlation spectroscopy — •Daniel Jürgens[1], Michael Uhrmacher[1], Ulrich Vetter[1], Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michel W. Barsoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil — [3]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

The compounds Zr_2InC and Hf_2InC belong to the class of MAX phases, which are known for their metallic and ceramic characteristics. Due to their unusual set of properties, these phases have been studied intensively in recent years with the aim to find new high-performance materials. Since most applied techniques only allow a macroscopic insight, the perturbed angular correlation (PAC) was used to determine the local environment of inserted probes on atomic scale. Radioactive ^{111}In and ^{181}Hf ions were implanted into the samples to measure characteristic electric field gradients, EFGs, at a certain site. The A-site EFG was investigated by using the ^{111}In isotope and the M-site by ^{181}Hf probes. In this study we report on the different annealing behaviors of In- and Hf-probes in Zr_2InC and Hf_2InC. We show that the A-site EFG strengths are nearly identical ($\nu_Q \approx 350\,\mathrm{MHz}$), while the EFGs for the M-site are unequal. We compare the experimental results with predictions from density functional theory calculations and give reasons why the A- and M-site EFGs are in such a way dissimilar.

MM 17.81 Mon 17:00 Poster B

The effect of the stacking sequence on the EFG in the MAX phase systems Ti-Al-X (X = C, N) — •Daniel Jürgens[1], Michael Uhrmacher[1], Ulrich Vetter[1], Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michel W. Barsoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil — [3]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

$M_{n+1}AX_n$ phases are nanolaminated layered ternary compounds and show both metallic and ceramic characteristics. These materials show an unusual set of properties and are therefore potential candidates e.g. for high-temperature applications. Most MAX phases belong to the 211 subclass (i.e. $n = 1$) and are made up of M_6X octahedra layers, which are separated from each other by one inserted A-layer. Only a few compounds exist with 312 (and 413) stoichiometry, where two (three) M_6X layers are embedded between two A-layers. The Ti-Al-C system is one among the few which can be synthesized in the 211 and 312 structure. For the Ti-Al-N system, the only stable compounds belong to the 211 and 413 classes.
By means of perturbed angular correlation (PAC), we measured the electric field gradients (EFGs) at the Al-site in these compounds. We could observe that the strength of the EFGs differ significantly between the different stacking sequences of the same system. In this contribution we show the experimental results and discuss the potential reasons for this effect.

MM 17.82 Mon 17:00 Poster B

2D quench calculations for FAIR Super-FRS dipole — •Piotr Szwangruber[1,2], Eric Floch[2], Thomas Weiland[1], and Oliver Boine-Frankenheim[1] — [1]Technische Universität Darmstadt, Institut für Theorie Elektromagnetischer Felder, Darmstadt, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

The Super Fragment Separator (Super-FRS) will be a part of the Facility for Antiproton and Ion Research (FAIR) placed in Darmstadt, Germany. Super-FRS will have superferric superconducting magnets working in liquid helium. Superconducting magnets need to be protected against quench (unwanted transition from superconducting to normal conducting state). To foresee the temperature distribution and voltage increase during a quench and to choose the best magnet protection system one needs to do the quench calculations before the first test of the magnet prototype.

This work presents a comparison between 2D quench calculations done on FAIR Super-FRS dipole with two different quench programs. The first was developed in GSI. It uses finite difference method and it is based on the heat equation. The second was a commercial FEM (FInite Element Method) software Opera 3D with the quench module. Obtained results are in good accordance between those programs.

MM 17.83 Mon 17:00 Poster B

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

The excellent physical properties of graphene make it a promising material for many scientific applications. The high electron mobility [1] and the relatively long spin lifetime [2] leading in spin diffusion lengths λ up to 2 microns [3], which make it a very interesting candidate for spintronics. By using of turbostratic graphene (TG), a multilayer of electronically decoupled graphene layers, one can overcome limits of λ like interaction between substrate and graphene as well as intrinsic corrugation in graphene sheets. TG combines the exciting properties of graphene with the higher robustness to environmental influences and the absence of inner corrugations of a microstructured material [4]. We present here successful spin injection from ferromagnetic electrodes into TG discs (in non-local spin valve configuration [3]) as well as transport properties of TG. [1] A. K. Geim et al., Nature Materials 6, 183 (2007), Science 324, 1530 (2009). [2] Hernando et al., Phys. Rev. B 74, 155426 (2006). [3] N. Tombros et al., Nature 448, 571 (2007). [4] M. Orlita et al., Phys. Rev. Lett. 101, 267601 (2008).

MM 17.84 Mon 17:00 Poster B

Ab initio-based mean field theory of site occupation in binary sigma phases — •Evgeniya Kabliman[1], Andrei V. Ruban[2], Oleg E. Peil[3], Peter Blaha[1], Karlheinz Schwarz[1], and Börje Johansson[2] — [1]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria — [2]Department of Materials Science and Engineering, Applied Material Physics, Royal Institute of Technology, Brinellvägen 23, SE-100 44 Stockholm, Sweden — [3]I. Institut of Theoretical Physics, Hamburg University, Jungiusstrasse 9, 20355 Hamburg, Germany

In present work we study the atomic site distribution in binary sigma-phases, which are found in many industrial alloys and usually lead to a destructive effect on the mechanical properties of these alloys. For this purpose we have proposed a simple and powerful approach to calculate

the site occupation numbers as function of temperature and composition [1,2]. It is based on the single-site mean-field description of the free energy, where the total energy is expanded in terms of on-site effective cluster interactions, which are calculated as relative chemical potentials. The suggested method has been successfully applied to the Fe-Cr, Co-Cr, Re-W and Fe-V sigma-phases.

[1] E. Kabliman, P. Blaha, K. Schwarz, A. V. Ruban, B. Johansson, Phys. Rev. B 83, 092201 (2011); [2] E. Kabliman, P. Blaha, K. Schwarz, O. Peil, A. V. Ruban, B. Johansson, Phys. Rev. B 84, 184206 (2011).

MM 17.85 Mon 17:00 Poster B

Ab-initio calculations of mechanical properties of TaxMo1-xN — •Khellil Bouamama — Laboratoire d'optoélectronique et composants, Université Ferhat Abbas, 19000 Sétif, Algeria

First-principles pseudopotential calculations of the lattice constants and of the mechanical properties for TaxMo1-xN alloys with B1-rocksalt structure were carried out. These calculations were performed using density functional perturbation theory (DFPT) within the virtual crystal approximation (VCA) for the disordered alloys and the supercell method (SC) for the ordered alloys. For the exchange-correlation potential the generalized gradient methods (GGA)is used. It is found that the addition of Mo induces a decisively ductile character in the clearly brittle TaN.

Keywords: Ab-initio, VCA, DFPT, nitride materials, elasticity

MM 17.86 Mon 17:00 Poster B

On the conductivity and chemical stability of lithium conducting glass ceramics (LICGC): Application in next generation batteries? — •Pascal Hartmann[1], Marisa Reich[2], Thomas Leichtweiss[1], Meike Schneider[2], Wolfgang Schmidbauer[2], and Jürgen Janek[1] — [1]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]SCHOTT AG, Corporate Research and Technology Development, 55014 Mainz, Germany

To fullfill future requirements in terms of electrical energy storage highly reactive materials will be used as active electrode components in the so-called next generation batteries. Most of the known liquid organic electrolytes decompose in contact with these materials making them not applicable. Therefore much effort has been spent to develop inorganic solid lithium electrolytes in order to protect the organic liquids or even completely replace them. One class of materials are glass ceramics. Especially the system $Li_{1+x}AlM(PO_4)_3$ (M = Ge, Ti,...) was intensively studied and it was claimed that these materials show a lithium ion conductivity of more than 1 mS/cm and that Ti-free samples, in addition, show good chemical stability upon reduction reactions. In this work we investigated glass ceramic materials with different ratios of Ge and Ti using electron microscopy, impedance spectroscopy, and low current polarization techniques. We show that there is a trend in terms of ionic conductivity, electronic conductivity and chemical stability upon the contents of Ge and Ti. These studies help to identify suitable material compositions to fulfill the requirements for long term stable and safe next generation batteries.

MM 17.87 Mon 17:00 Poster B

A new 2D-ACAR spectrometer at the NEPOMUC positron facility — •Hubert Ceeh[1], Josef Weber[1], Christoph Hugenschmidt[1,2], Michael Leitner[3], and Peter Böni[1] — [1]Technische Universität München E21, Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Garching, Germany — [3]Technische Universität München E13, Garching, Germany

The 2D-ACAR (Angular Correlation of Annihilation Radiation) technique is a well suited method for the investigation of the electronic structure, in particular the fermiology of correlated systems. Measuring the two dimensional projection of the two-photon-momentum-distribution of the annihilation radiation the three dimensional electron momentum distribution can be calculated via tomographic reconstruction. A new 2D-ACAR spectrometer is currently being installed at the NEPOMUC facility at the research reactor in Garching. In the setup, the positrons from a 50 mCi ^{22}Na source are guided onto the sample by an axial magnetic field created by a normal conducting electromagnet. The use of especially developed soft iron pole caps, guarantees a homogeneous magnetic field with a magnetic flux density > 1.2 T while allowing axial access to the sample- and positioning stage. The sample stage itself can be cooled by a standard cryo-cooler to temperatures below 30 K in order to reduce the smearing of the angular resolution by the positron momentum. The key features of the new spectrometer are presented. In addition, first results of measurements on a intermetalic Heussler crystal are discussed and compared with first principle band structure calculations.

MM 17.88 Mon 17:00 Poster B

The effect of grain size and grain boundaries on the mechanical behaviour of MAX phases — •Thilo Seliger[1], Cynthia Volkert[1], Christoph Brüsewitz[2], Hans Hofsäss[2], and Michael Uhrmacher[2] — [1]Institut für Materialphysik, Universität Göttingen, D-37073 Göttingen — [2]II. Physikalisches Institut, Universität Göttingen, D-37073 Göttingen

It is well known that the MAX phases (layered ternary carbides and nitrides) have unusual mechanical properties. They exhibit features from both metals (machinable, damage tolerant, good thermal and electrical conductivities) and from ceramics (high stiffness and low thermal expansion). This is attributed to the fact that dislocations only move on a single set of parallel planes, which results in kinking and shear band formation during deformation. It has been observed that the formation of kinks and shear bands is influenced by the grain size, leading to an increase in strength with decreasing grain size. We seek to take advantage of the grain size dependent strength and the damage tolerance of the MAX phases to explore the possibility of designing nanocrystalline MAX phases with both high strength and high ductility. We investigate the effect of grain size and individual grain boundaries on the nanoindentation response of Ti-based bulk MAX phases. A combination of EBSD to determine grain orientations, focused ion beam to mark specific locations and Berkovich nanoindentation have been used. The relation between local mechanical properties and local microstructure will be presented and discussed and used to develop guidelines for optimum grain sizes and textures.

MM 17.89 Mon 17:00 Poster B

Advanced EBSD/EDS integration for efficient and modern materials characterization — Daniel Goran, Laurie Palasse, and •Thomas Schwager — Bruker Nano GmbH, Schwarzschildstrasse 12, 12489, Berlin, Germany

Recent software and hardware developments have greatly increased the speed at which simultane-ous Electron BackScatter Diffraction (EBSD) and Energy Dispersive X-Ray Spectroscopy (EDS) mapping can be done. We will demonstrate that new developments have transformed the combina-tion of these techniques into a powerful tool for characterizing multiphase materials with improved efficiency and data quality, introducing new ways of using the two complementary techniques to ensure data integrity.

It is well known that the information delivered either by EBSD or by EDS alone is not enough to successfully distinguish the different phases present, like for phases creating similar patterns or sim-ilar chemical composition. Typical examples are quartz and cristobalite, rutile and magnetite.. The new approach consists of simultaneously acquiring an EBSP and a complete EDS spectrum for each point in the map (up to 500 points/sec), then a two-step online/offline analysis method can be used to automatically discriminate phases creating similar patterns using the quantified EDS results to decide or narrow down the phase in each point, finding the correct crystallographic orientation for that particular point. Moreover, if one or more unknown/unexpected phases are present, the EDS information can be used for offline phase identification (up to 54000 points/sec).

MM 18: HV Kraft

Time: Tuesday 9:30–10:00 Location: H 0107

Invited Talk MM 18.1 Tue 9:30 H 0107

Twinning-mediated plasticity in Au Nanowires — Andreas Sedlmayr[1], Reiner Mönig[1], Gunther Richter[2], and •Oliver Kraft[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology — [2]Max-Planck-Institut for Intelligent Systems, Stuttgart

We have developed an experimental method for the mechanical characterization of nanowires with diameters between 30 and a few hundred nanometers. The setup is used inside a dual beam SEM/FIB, and stress-strain curves are measured using piezoelectric actuators and a three-plate capacitor based transducer for applying and measuring force. High resolution strain data is obtained by digital correlation of the SEM images. In this paper, we report on the deformation behavior of Au nanowires, which were produced by a physical vapor deposition process. The nanowires are single crystal with [110]-orientation, and initially free of defects such as dislocations or growth twins. The stress-strain data show strengths exceeding 1 GPa and plastic strains of the order of 10% without a clear size dependence in the regime investigated. The in situ SEM observations show that the deformation is governed by twinning which occurs in two distinct modes. Moreover, the measured strength values show a large scatter indicating that the deformation process may be influenced by the statistical occurrence of small flaws, most likely at the nanowire surface, triggering the onset of deformation.

MM 19: Computational Materials Modelling IV - Finite Temperature

Time: Tuesday 10:15–12:00 Location: TC 006

MM 19.1 Tue 10:15 TC 006

Interfacial free energy calculations via direct thermodynamic integration across phase boundaries — •Paul Erhart[1,2] and Babak Sadigh[2] — [1]Applied Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Lawrence Livermore National Laboratory, Livermore, California, USA

We present a general technique for constraining macroscopic fluctuations in thermodynamic variables well-suited for Monte Carlo simulations of multiphase equilibria. In particular for multicomponent systems this amounts to an extension of the semi-grand canonical ensemble (SGC), the so-called variance-constrained (VC) SGC ensemble. It allows for Monte Carlo simulations of multiphase equilibria and thermodynamic integration across phase boundaries, from which equilibrium free energies of multiphase systems can be obtained. We apply this method to calculate alpha/alpha' interface free energies in Fe-Cr alloys as a function of orientation and temperature.

MM 19.2 Tue 10:30 TC 006

Fully ab initio determination of anharmonic contributions by efficient sampling strategies — •Albert Glensk[1], Blazej Grabowski[2], Tilmann Hickel[1], and Joerg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung — [2]Lawrence Livermore National Lab

Using ab initio approaches, temperature dependent thermodynamic free energies are nowadays typically calculated within the quasiharmonic approximation. Numerically highly accurate ab initio calculations for Al including anharmonic contributions on the other hand showed a significant change in the heat capacity and a dramatic effect on the entropy of vacancy formation in Al compared to quasiharmonic results [1]. By developing and implementing highly efficient sampling methods, we are now able to routinely determine anharmonic contributions for metals. Using these methods we were able to systematically improve the ab initio based thermodynamic description of Al-Mg-Si-Cu alloys. Particularly, the influence of anharmonicities on the unary subsystems of these alloys, consequences for the phase diagrams and deviations from quasiharmonic results will be discussed.

[1] B. Grabowski et al, PRB 79, 134106 (2009)

MM 19.3 Tue 10:45 TC 006

Analysing reaction coordinates and free energies for phase transformations within the reweighted path ensemble — •Jutta Rogal and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Sampling rare events in complex, high dimensional systems, such as crystal nucleation and growth, remains a challenge for computational studies. Employing e.g. classical molecular dynamics simulations to model phase transformations with a sizeable nucleation barrier becomes quickly unfeasible as the system tends to spend most of the time within the stable states while it hardly samples the transition barrier regions of the phase space.

Among other approaches, transition path sampling (TPS) provides a possibility to explore transitions between stable states in rare event systems. One of the key advantages in TPS is that an a priori definition of a reaction coordinate is not required. And by using the underlying physical dynamics the true kinetics of the transition is sampled.

Here we introduce a reweighting scheme for the path ensembles and apply it to a solid-liquid phase transformation in a Lennard-Jones model system. Once the sampling has been performed, the reweighting allows for the analysis of free energy surfaces and committor projections in an arbitrary order parameter space. The reweighted path ensemble can then be used to optimise non-linear reaction coordinates and extract parameters such as the solid-liquid interface free energy, which is one of the key quantities governing nucleation and growth during solidification.

MM 19.4 Tue 11:00 TC 006

Ab initio **study of elasticity and phase transformations in Fe above the Curie temperature** — Martin Friák[1], •Alexander Udyansky[1], David Holec[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Montanuniversität Leoben, Leoben, Austria

Understanding and tailoring the thermodynamic and elastic properties of paramagnetic body-centered cubic iron (β-Fe) is fundamental for developing Fe-based materials operating at elevated temperatures. We have therefore studied β-Fe, modeled by an antiferromagnetic supercell, with the internal distribution of local magnetic moments having the special quasirandom structure (SQS). In contrast to previously suggested antiferromagnetic models that were found to be mechanically unstable with respect to tetragonal deformations, the proposed SQS supercell is stable. Using this approach the thermodynamic stability of β-Fe with respect to tetragonal and trigonal deformations has been studied. The corresponding total energies have been determined for a broad range of deformations and are compared with those calculated for other magnetic states. The calculated single-crystalline elastic constants are found to closely reproduce experimental data detected within the temperature range of β-Fe.

MM 19.5 Tue 11:15 TC 006

Wall-liquid and wall-crystal interfacial excess free energies via thermodynamic integration: A molecular dynamics simulation study — •Ronald Benjamin and Juergen Horbach — Institut für Theoretische Physik II, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany

A method is proposed to compute the wall-liquid and wall-crystal interfacial excess free energy by molecular dynamics simulation. Our approach is based on a thermodynamic integration scheme, where the wall-liquid (or wall-crystal) interaction potential is gradually modified so that we move from a reference state of known interfacial energy to the state of interest and then computing the difference in the Gibbs excess free energy. We test our method by applying it to a Lennard Jones (LJ) system in contact with a wall, which is either flat or structured. The flat wall is modeled by a WCA potential and the structured wall consists of a few layers of particles rigidly fixed at the sites of an ideal fcc crystal lattice and interacting with the liquid (crystal) via the LJ potential. The interfacial excess energy is also determined from the stress anisotropy and we find good agreement between the two

approaches.

MM 19.6 Tue 11:30 TC 006

The solubility of oxygen in HCP-Ti revisited on the basis of first-principles calculations — •Paul Erhart[1] and Mark Asta[2] — [1]Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Materials Science and Engineering, University of California, Berkeley

Most experimental and computed phase diagrams for the Ti–O system indicate a very large solubility of O of up to 30% in hexagonal closed packed (HCP) Ti at low temperatures. Yet already much smaller amou nts of oxygen on the order of just fractions of a percent are known to cause rather dramatic changes of the mechanical properties, most notably the ductility. Using a combination of first-principles calculations and Monte Carlo simulations based on lattice Hamiltonians, we have systematically investigated the Ti-rich end of the Ti–O phase diagram. The simulations predict three distinct Ti–O phases that are based on the HCP lattice: Ti_6O, Ti_3O, and Ti_2O. The structures of these phases are in exact agreement with the results of neutron diffraction experiments that hitherto have been integrated incompletely or not at all into available phase diagrams. Using our approach we obtain a revised equilibrium phase diagram in the concentration range up to 33% oxygen. Our results show that the effectice equilibrium solubility of O in Ti is fact less than 1% at room temperature. Beyond this concentration excess oxygen precipitates in the form of Ti_6O. We suggest that the Ti_6O regions effectively lead to a form of precipitation hardening (as opposed to solution hardening) and thus have an important effect on dislocation motion and plasticity.

MM 19.7 Tue 11:45 TC 006

Point defect interactions of boron in α-Fe — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Bochum, Germany

Modern steels are multicomponent systems that combine iron and carbon with further elements in order to achieve specific properties. The effect of boron additions depends on their spatial distribution that are affected not only by the fabrication process but also by interactions with other constituents. The latter may result in boron redistribution or the formation of boron-containing precipitates. In order to gain insight into the interaction of boron with point defects and impurities within the host matrix, we performed ab-initio calculations based on density functional theory for the case of α-Fe. We determined the distance-dependent interaction energies for different point defects, in particular a second boron atom, a vacancy and borons' nearest neighbours in the periodic table: carbon, nitrogen and oxygen atoms. We observe that the interaction tendency is primarily determined by the position of boron, and virtually independent of the second point defect: substitutional boron binds the second point defect, while interstitial boron repels it.

MM 20: Topical Session Bulk Nanostrucured Materials IV - Microstructure and Characterization II

Time: Tuesday 10:15–11:30 Location: H 0107

Topical Talk MM 20.1 Tue 10:15 H 0107

Stabilisation of nanocrystalline materials by defects — •Harald Rösner — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany

The stability of nanocrystalline materials is an important issue and of technological interest. Grain growth occurs in polycrystalline materials to reduce the grain boundary area and hence the total energy of the system. Therefore, the high density of interfaces in nanocrystalline materials is likely to provide a significant driving force for grain growth. However, grain growth can be suppressed by the presence of either impurities or defects. In this talk a comprehensive study of defect-stabilized nanocrystalline Pd using aberration-corrected transmission electron microscopy is presented. Local strains were quantified at grain interiors and interfaces (grain/twin boundaries, triple/quadruple junctions) using the geometric phase analysis; a technique that allows calculation of the in-plane components of the strain tensor. The results obtained suggest that rotational defects play a significant role as stabilising elements for nanocrystalline structures.

MM 20.2 Tue 10:45 H 0107

Quantitative grain size and twin density analysis by TEM-OIM measurements for tensile testing of nanocrystalline Pd — •Aaron Kobler[1,2], Anna Castrup[1,2], Christian Kübel[1], and Horst Hahn[1,2] — [1]Institute of Nanotechnology (INT/KIT), Eggenstein, Germany — [2]Joint Research Laboratory Nanomaterials (KIT and TUD), Darmstadt, Germany

To study the deformation mechanisms in nanocrystalline (nc) Pd, we performed tensile tests on magnetron sputtered thin films in combination with orientation imaging (OIM) analysis in a TEM. TEM-OIM is a new technique that fills the gap of EBSD measurements for grain sizes below 30-50 nm. We have implemented the OIM (NanoMegas) on a FEI Tecnai F20 in micro-probe (up) STEM mode, that allows us to acquire (fast) STEM reference images. Once an OIM map is acquired, the grain size and twin density is evaluated using Mtex. The main advantage of this approach is a much better identification of grains and sub-grains and the detection of all twin boundaries within the area of interest. The thin films were magnetron sputtered onto Kapton films to avoid strain localization using conditions previously identified to minimize growth induced residual stress. Subsequently, the films were individually deformed in tension up to 0%, 2%, 3,5%, 5% and 10% and prepared for TEM imaging. Our evaluation based on the BF/DF-TEM and OIM reveals qualitatively similar results and show that the grain size and the twin density both increase continuously with increasing strain. However, the absolute twin density observed by OIM is significantly higher compared to DF-TEM as almost all twins are detected.

MM 20.3 Tue 11:00 H 0107

Electron microscopic studies of Ni_3Ge deformed by high pressure torsion — •Andreas Grill, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

Nanocrystalline $L1_2$ ordered intermetallics processed by high pressure torsion (HPT) show improved mechanical properties [1]. The persistance of larger grains oriented for multiple slip embedded in the nanocrystalline structure indicates that highly symmetric orientations are less favourable to form nanograins [2]. To study the evolution process of nanocrystallization as a function of orientation single crystalline $L1_2$ ordered Ni_3Ge of two different initial orientations was deformed by HPT. The structure of the samples was investigated by electron microscopy methods. At low numbers of turns electron backscatter diffraction of the cross section of the HPT discs shows homogeneous fragmentation. At higher numbers of turns bands are formed inhomogeneously. They cross the fragmented matrix and accumulate near the top and bottom surfaces. Transmission electron microscopy studies show that the bands consist of elongated nanograins whereas the neighbouring regions are fragmented crystallographically by a high density of defects accumulating on highly activated {111} glide planes. Finally, in the present case the different orientations seem to have little influence on the deformation structures.

[1] K. Tsuchiya, O. Ciuca. Mat. Sci. For. 667-669, 17 (2011). [2] C. Rentenberger, H. P. Karnthaler. Int. J. Mat. Res. 98, 4 (2007). This work was supported by the Austrian Science Fund (FWF): [P22440].

MM 20.4 Tue 11:15 H 0107

Texture evolution in NiAl deformed by high pressure torsion — •Christine Tränkner[1], Robert Chulist[1], Werner Skrotzki[1], Benoit Beausir[2], Thomas Lippmann[3], Jelena Horky[4], and Michael Zehetbauer[4] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux (LEM3), Université Paul-Verlaine de Metz, Metz-57012, France — [3]Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — [4]Fakultät für Physik, Universität Wien, Austria

Small discs of polycrystalline NiAl were deformed by high pressure tor-

sion at temperatures from room temperature up to 500°C and pressures ranging from 2 to 8 GPa. In this way, very high local shear strains at the edge of the samples of about 70 could be achieved. Local textures were measured by high-energy synchrotron radiation at several positions from the centre to the edge of the samples. Due to increasing shear strain along this line a texture gradient is observed. The texture also changes with processing temperature and pressure. Type and intensity of texture will be discussed with respect to slip system activity and recrystallization.

MM 21: Microstructure and Phase Transformations II

Time: Tuesday 10:15–11:45 Location: H 0106

MM 21.1 Tue 10:15 H 0106

A phase-field simulation of directional solidification in ternary Al-Cu-Ni alloys — •Julia Kundin[1], Henning Hörstermann[1], Rainer Schmid-Fetzer[2], and Heike Emmerich[1] — [1]Material- und Prozesssimulation, Universität Bayreuth, 95448 Bayreuth, Germany — [2]TU Clausthal, Institute for Metallurgy, 38678 Clausthal-Zellerfeld, Germany

A precise calculation of the directional solidification based on a reliable thermodynamic description is carried out in a ternary Al-Ci-Ni alloy. A comprehensive understanding of the interplay between the phases in the three-phase peritectic reaction and in the four-phase transition reaction, and their influence on the nucleation kinetics and the resulting microstructure evolution is of great interest. A three-phase peritectic reaction in a ternary system is no longer invariant but a univariant reaction, which means, the equilibrium compositions of all phases vary with the temperature. For a four-phase reaction $L + \alpha \rightarrow \beta + \gamma$, there are two product phases, which have an effect on the nucleation. If the product phase β first precipitates via heterogeneous nucleation on the primary phase α, these precipitates of β may be also a potent nucleant for the other product phase γ. The microstructure formation of a ternary Al-Cu-Ni alloy during the directional solidification with a three-phase peritectic reaction and a four-phase transition reaction is simulated by a quantitative multi-phase multi-component phase-field model. The refined thermodynamic description of the system as well as other input data for the phase-field model are discussed.

MM 21.2 Tue 10:30 H 0106

Comparative investigation of phase-field models based on free energy and grand potential formulations — •Oleg Tschukin[1], Abhik Choudhury[2], and Britta Nestler[1,2] — [1]IMP - Hochschule Karlsruhe Technik und Wirtschaft — [2]IAM - Zuverlässigkeit von Bauteilen und Systemen, Karlsruher Institut für Technologie

We present a comparison between a phase-field model for multi-component solidification based on a grand potential functional constructed out of the thermodynamic chemical potential μ: $f\left(c\left(\mu,T\right),T\right)-\mu c\left(\mu,T\right)$[1] and the free energy functional of the average concentration [2]. Contrary to formally used free energy functionals, when the evolution equations are derived from the grand potential formulation, there exist certain advantages: length scales of simulations can be upscaled and surface as well as kinetic properties can be easily calibrated. We perform a quantitative evaluation of both methodologies by applying them to common problems of multi-phase solidification (eutectic and peritectic solidification). While both methods can be used to derive the same physics, we point out the efficiencies and advantages of the grand potential formalism.

[1] A. Choudhury *et al.*: Grand potential formalism for multi-component phase transformations along with thin-interface asymptotics of the double obstacle potential, submitted to Physical Review E (2011)

[2] H.Garcke *et al.*: A diffuse interface model for alloys with multiple components and phases, SIAM J Appl. Math. 64 775-799 (2004)

MM 21.3 Tue 10:45 H 0106

A phase-field study of morphology effects in heterogeneous nucleation — •Henning Hörstermann, Julia Kundin, and Heike Emmerich — Material- und Prozesssimulation, Universität Bayreuth, 95448 Bayreuth, Germany

The effect of the morphology of the primary phase on heterogeneous nucleation in peritectic materials is studied using a quantitative phase-field method on an example of an Al-Ni peritectic alloy based on the refined thermodynamic data related to the Gibbs energies of the phases. The nucleation energy barrier of the peritectic Al_3Ni_2 phase is estimated by determining the critical nucleus radius in three dimensions for different shapes and curvatures of the primary Al_3Ni seed. The undercooling of the peritectic reaction used in the simulations was taken from DSC experiments. The nucleation energy and the contact functions calculated from the phase-field simulations are compared to predictions from classical nucleation theory.

MM 21.4 Tue 11:00 H 0106

Abnormal grain growth of Goss grains in grain-oriented electrical steel — •Wei Guo[1] and Wei-min Mao[2] — [1]Department of Microstructure Physics and Alloy Design,Max-Planck Institute for Iron Research GmbH, Duesseldorf, Germany — [2]2, School of Materials, University of Science and Technology, Beijing, Beijing, China

Strong Goss texture {110}<001> in grain-oriented electrical steels forms by abnormal grain growth during high temperature recrystallization annealing. However, the cause of this abnormal growth has been disputed for more than 70 years. The various explanations include high fraction of high angle boundaries, high mobility of coincidence site lattice boundaries, size effects and so on. However, none of these explanations address the internal environment of Goss oriented grains. Here we use electron back scattering diffraction techniques and field emission microscopy to show that some Goss oriented grains in matrix have higher secondary particle densities than their neighbors during final annealing at 875 degree C before secondary recrystallization. Since regions with higher second phase particle density offer a high resistance to grain boundary migration, Goss oriented grains ought to grow more readily towards regions with lower secondary particle density. Therefore, we conclude that second phase particle densities must play a vital role in the growth of Goss oriented grains. This findings may shed light on optimizing Goss texture and improve magnetic properties of grain oriented electrical steels.

MM 21.5 Tue 11:15 H 0106

Investigation of Grain Growth in $SrTiO_3$ by diffraction contrast tomography and modelling — •Daniel Weygand[1], Melanie Syha[1], Wolfgang Rheinheimer[1], Wolfgang Ludwig[2], Erich Lauridsen[3], and Peter Gumbsch[1,4] — [1]KIT, IAM, Karlsruhe, Germany — [2]ESRF, Grenoble, France — [3]Risoe National Lab., Roskilde, Denmark — [4]IWM, Freiburg, Germany

The grain growth dynamics of bulk $SrTiO_3$ samples have revealed a puzzling growth behaviour, the sudden decrease of the growth rate with increasing temperature [1]. Metallographic analysis of two-dimensional sections through the bulk samples has not revealed any specific quantities, related to this growth acceleration.

Therefore diffraction contrast tomography measurements and subsequent reconstructions of the three dimensional grain structures in $SrTiO_3$ and three dimensional grain growth modelling have been employed to characterize the grain structure. Samples have been analysed at different states of the heat-treatment. This allows determining the growth dynamics of specific grains, knowing the geometry and crystallographic orientations of the surrounding grains.

[1] Bäurer, M., Weygand, D., Gumbsch, P. and Hoffmann, M.J.: Grain growth anomaly in strontium titanate, Scripta Mat. 61 (2009),584.

[2] M. Syha, W. Rheinheimer, M. Bäurer, E.M. Lauridsen, W. Ludwig, D. Weygand, P. Gumbsch, Three-dimensional grain structure of sintered strontium titanate from X-ray diffraction contrast tomography, Script Mat. 66 (2012) 1.

MM 21.6 Tue 11:30 H 0106

Measuring dihedral angles in polycrystalline grain microstructures — Stefan Schäfer and •Dana Zöllner — Abteilung Materialphysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität, 39106 Magdeburg

Dihedral angles in polycrystalline grain microstructures are known to control the morphology of the structure and therewith also the microstructural evolution during grain growth. Hence they play an im-

portant role in grain growth theories, but are rarely measured. For exact measurements two problems have to be considered. First, assumptions have to be made regarding the shape of the grain boundaries and their triple junctions. Secondly, in digital discretised grain microstructures grain boundaries usually do not have a physical representation in the images but are defined to be between two grains of unlike orientation and are - due to the use of pixels in 2D and voxels in 3D - not smooth but rather staircase-shaped.

In this work we discuss a method to measure dihedral angles in two and three dimensional discretised (digital) grain microstructures based on trisections of circles resp. spheres. Measuring errors are examined and the method is applied to grain structures obtained by Monte Carlo Potts model simulations.

MM 22: Functional Materials I

Time: Tuesday 10:15–11:30 Location: H 1029

MM 22.1 Tue 10:15 H 1029

Optimizing thermoelectric Properties: Microstructure Analysis of $AgPb_{18}SbTe_{20}$ — •Susanne Perlt[1], Thomas Höche[2], Jayaram Dadda[3], and Eckhard Müller[3] — [1]Leibniz Institute of Surface Modification, Leipzig — [2]Fraunhofer Institute for Mechanics of Materials, Halle — [3]German Aerospace Center, Institute of Materials Research, Köln

Given the looming shortage of natural resources, there is a growing interest in renewable energy in recent years. The feasible recovery of waste-heat energy as it is generated by industrial and vehicle engines has led to increasing research interest in thermoelectrics (TE). In order to get TE materials with high performance, i.e. with a large figure of merit ZT, one needs to tune electronic and phononic properties. A promising candidate is the quaternary compound $AgPb_mSbTe_{2+m}$ (Lead-Antimony-Silver-Tellurium, LAST-m). Its excellent performance is mainly based on a low value of the thermal conductivity κ - widely believed to be caused by self-assembled nanostructures. This study reports microstructure investigations at two different length scales. The micrometer scale was evaluated by SEM to analyze volume fraction and number of secondary phases as well as the impact of processing parameters on the homogeneity of bulk samples. Site-specific liftout of TEM lamellae from thermoelectrically characterised samples was made to investigate the structure on the nanometer scale. High-resolution TEM was performed to reveal shape and size distribution of nanoprecipitates. An attempt is made to derive a structure-property relationship.

MM 22.2 Tue 10:30 H 1029

Reference materials for traceable measurements of thermoelectric properties from 300 K to 900 K — Frank Edler[1], •Ernst Lenz[1], and Pawel Ziolkowski[2] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]German Aerospace Center - Institute of Materials Research, Germany

Thermoelectric generators for converting wasted heat directly into electric energy are of increasing interest during the last years. The efficiency of those generators is normally expressed by the dimensionless figure of merit which scales with the square of the Seebeck coefficient. However, traceable reference materials for Seebeck coefficients in the temperature range of 300 K to 900 K are still not available. The intention of the project "Metrology for Energy Harvesting" founded by the European metrology organization is to provide those reference materials [1].

A metallic nickel copper alloy (CuNi44) and a semiconducting iron disilicide ($Fe_{0.95}Co_{0.05}Si_2$) will be presented as two possible reference materials. A relative uncertainty of about 2% for the Seebeck coefficient can be shown under utilization of an improved measurement system. The enhancement of the measuring system will be achieved by using gold/platinum thermocouples and a Pt-100 thermometer.

[1] http://www.empronline.eu/energycall/index.html

MM 22.3 Tue 10:45 H 1029

First-principles study of native point defects in the thermoelectric material Bi_2Te_3 — •Adham Hashibon and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

The thermoelectric properties of Bi_2Te_3, which is the currently preferred thermoelectric material for energy conversion applications at room temperature, are strongly affected by the nature and concentration of native point defects. However, knowledge of the formation energies of point defects and the manner by which they affect thermoelectric properties is still incomplete. We present a systematic study of formation energies and electronic densities of states for native point defects in Bi_2Te_3 [1] using first-principles calculations based on density functional theory. Formation energies are calculated assuming the dilute limit of defects by employing an ab-initio thermodynamics approach. Results for the formation energies of the most prominent native point defects, namely vacancies and anti-site defects on the Bi, Te1, and Te2 sub-lattices of the Bi_2Te_3 structure will be presented and their impact on the thermoelectric properties will be discussed.

[1] Adham Hashibon and Christian Elsässer, Phys. Rev. B 84, 144117 (2011)

MM 22.4 Tue 11:00 H 1029

Dynamic stabilisation of polar oxide growth: the case of MgO(111) — •Philip Hasnip and Vlado Lazarov — University of York, York, UK

Intrinsic polar materials such as metal-oxides are some of the most commonly used materials in electronic, magnetic and chemical applications. Along the polar direction, these materials consist of oppositely charged ionic planes and this polarity dominates the growth process. Attempts to grow polar oxides in their polar direction often result in surface faceting, surface reconstructions, adatoms or surface metallisation as the system attempts to heal the polarity and prevent a divergent electrostatic dipole.

By using MgO(111) as a model system for polar oxide film growth, we show by ab initio calculations that H can act as a surfactant, stabilising the growth dynamically without disrupting the growth or becoming trapped in the film. The continuous presence of H during the growth of a MgO(111) film efficiently removes the microscopic dipole moment, thus enabling the growth of perfect fcc-ordered MgO(111) films. These theoretical predictions are confirmed experimentally by molecular beam epitaxy single crystal growth of MgO(111) on SiC(0001).

MM 22.5 Tue 11:15 H 1029

Three displacively excited coherent phonons in infinite BN nanotubes — •Bernd Bauerhenne, Eeuwe Zijlstra, and Martin Garcia — Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

BN nanotubes are isostructual to carbon nanotubes with boron and nitrogen atoms occupying the even and odd sublattices, respectively. They are described by the so called wrapping vector, which defines how the hexagonal sheet is cut off and rolled up. The wrapping vector also divides the tubes into the three groups: armchair, zizag and chiral. In particular, we investigate the excitation of a (5,0) zigzag BN nanotube with an intense ultrashort laser pulse by means of ab initio molecular dynamics simulations on laser-excited potential energy surfaces. Our results show that only three phonon modes are simultaneously excited. We identify these three modes as the radial breathing mode, the radial buckling mode and the longitudinal bond stretching mode. The frequencies of the three modes show a softening for increasing laser intensity. The analysis of our results show, that we can describe all effects of the laser excitation by a three-dimensional harmonic oscillator. Using this model we analyse the possibility to steer the excitation of the three modes by using, instead of one, two or three pump laser pulses.

MM 23: Topical Session Bulk Nanostrucured Materials V - Microstructure and Characterization III

Time: Tuesday 11:30–13:00 Location: H 0107

MM 23.1 Tue 11:30 H 0107

X-ray line profile analysis of in-situ tensile deformation experiments of nanocrystalline palladium thin films — •Michael Kerber[1], Patric Gruber[2], Rudolf Baumbusch[2], Jochen Lohmiller[2], Anna Castrup[3], Erhard Schafler[1], Oliver Kraft[2], Michael Zehetbauer[1], and Horst Hahn[3] — [1]University of Vienna, Physics of Nanostructured Materials, Vienna, Austria — [2]Karlsruhe Institute of Technology IAM II, Eggenstein-Leopoldshafen, Germany — [3]Karlsruhe Institute of Technology INT, Eggenstein-Leopoldshafen, Germany

X-ray line profile analysis was used to study the evolution of the microstructural parameters in Pd with grain sizes around 30nm. The Pd-films of about 1 μm thickness were produced by sputtering of Pd onto a Kapton foil. X-ray profiles were measured during the tensile deformation at the MS-beamline of the synchrotron SLS, Villigen (Switzerland) at deformation temperatures of 20° C and 60° C. The samples were loaded/unloaded in two consecutive cycles to $\epsilon \sim 0.2$ and 0.4. The evaluation of the data yielded the detailed evolution of the median m and variance σ of an assumed log-normal size-distribution, the density of dislocations ρ and their arrangement M, and the frequency of planar defects β. The changes in the diffuse background scattering, related to the number of point defects of the material, was determined. Here it was found that the deformation is still ruled by dislocation plasticity. However, grain size mediated deformation gets increasingly active, and effects from vacancies play some role. Part of the Work supported by the Austrian Science Fund project S 10403

MM 23.2 Tue 11:45 H 0107

Nano crystallization in glasses, their structure and chemistry as analyzed by anomalous small angle X-ray scattering — •Vikram Singh Raghuwanshi[1], Armin Hoell[1], Ruzha Harizanova[2], and Christian Rüssel[3] — [1]Helmholtz Zentrum Berlin für Materialian und Energie, Berlin, Germany — [2]University of Chemical Technology and Mateallurgy,Sofia,Bulgaria. — [3]Otto-Schott-Institut,Jena, Germany

Silicate glasses containing nano crystals have valuable applications in various fields. The aim is to estimate the structural parameter and composition of the nanostructure embedded in silicate glass system by SAXS and ASAXS. We have chosen two silicate systems. Firstly, glass ceramics having composition 62.9SiO2/13.6Na2O/8.5MnO/15.0Fe2O4-x (mol %) and by applying time/temperature heat treatment regime, nano-sized crystalline phase of MnxFe1-xFe2O4 is precipitated. ASAXS measurements were performed near the Fe and Mn K edge. Secondly, glass ceramics having composition 69.6SiO2/7.5Al2O3/15.0K2O/1.9Na2O/4BaF2/2BaO (mol %) shows precipitation of BaF2 nanocrystals during controlled annealing at different time/temperature scales. ASAXS measurements were performed near the Ba L3 edge. Fitting of ASAXS curve shows the formation of spherical particles surrounded with Si enriched lower electron density layer. This layer acts as a diffusion barrier and due to which, further growth of the nanoparticles is kinetically constraint. Also quantitative information and composition of the particles is evaluated.

MM 23.3 Tue 12:00 H 0107

Following deformation mechanisms in nanocrystalline Ni and PdAu using diffraction techniques — •Patric Gruber[1], Jochen Lohmiller[1], Oliver Kraft[1], Christian Braun[2], Manuel Grewer[2], Rainer Birringer[2], Kerstin Schüler[2], Aaron Kobler[3], Christian Kübel[3], and Veijo Honkimäki[4] — [1]KIT, Institute for Applied Materials, Karlsruhe — [2]Universität des Saarlandes, Saarbrücken — [3]KIT, Institute of Nanotechnology, Karlsruhe — [4]ESRF, Grenoble, France

The contribution of specific deformation mechanisms which have been proposed for nanocrystalline (nc) materials is still under heavy debate. In situ characterization is necessary in order to (i) detect reversible mechanisms and (ii) ascribe the active mechanism to the respective strain regime. Therefore in situ compression tests are conducted on nc Ni and PdAu specimens using high energy synchrotron X-ray diffraction (XRD). Alloying of Au to Pd is expected to strongly influence the different deformation mechanisms of nc Pd and consequently give new insight in the predominant deformation mechanisms of nc materials in general. Based on the in situ experiments the deformation behavior of nc Ni and PdAu can be determined to be a distinct sequence of elastic grain interaction, grain boundary sliding, grain rotation, dislocation activity and grain growth. The succession of the different deformation mechanisms leads to a specific in-plane texture which could be determined for the first time. The specific differences in deformation behavior for Ni and PdAu alloys with varying Au content will be discussed.

MM 23.4 Tue 12:15 H 0107

Elemental distribution and solid solubility of nanocrystalline near-equilibrium Fe and Cu alloys — •Thomas Riedl[1], Alexander Kirchner[1], Konrad Eymann[1], Ralf Schlesiger[2], Ahmed Shariq[3], and Bernd Kieback[1] — [1]Institut für Werkstoffwissenschaft, TU Dresden, 01062 Dresden, Germany — [2]Institut für Materialphysik, Univ. Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [3]Fraunhofer-Center für Nanoelektronische Technologien, Königsbrücker Str. 180, 01099 Dresden, Germany

Nanocrystalline (nc) alloys exhibit a large volume fraction crystallite interface regions, notably grain boundaries (GBs) [1]. Owing to the reduced atom density GBs can offer favourable sites for solute atoms. In the present work we investigate the solid solubility of nc near-equilibrium bcc Fe and fcc Cu matrices for conventionally immiscible solutes. As preparation route the mechanical alloying technique followed by annealing was selected. Atom probe tomography analyses show that Mg and C solute atoms are enriched in the GBs of 12nm grain sized Fe. From that, segregation strengths and solute interaction parameters are derived. Complementary to the experimental study thermodynamic calculations of solid solubilities have been performed [2,3].

[1] H. Gleiter: Prog. Mater. Sci. 33 (1989) 223
[2] A. Kirchner and B. Kieback: Scr. Mater. 64 (2011) 406
[3] Financial support by the Deutsche Forschungsgemeinschaft via the Emmy-Noether program is appreciated.

MM 23.5 Tue 12:30 H 0107

Metallic Nanoglasses: Structure, Stability and Mechanical Properties — Karsten Albe[1], •Yvonne Ritter[1], Daniel Sopu[1], and Herberg Gleiter[2] — [1]TU Darmstadt, FB Material- und Geowissenschaften, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt — [2]KIT, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen

Grain boundaries are defined as 2-dimensional planar defects in crystalline materials. For the case of glasses, in contrast, there is no established concept of grain boundaries. If one considers, however, that a high degree of short- and medium-range order is also found in glassy materials, the definition of a grain boundary in a glass as an internal interface enclosing a domain of atoms becomes conceivable. Moreover, in bulk metallic glasses (BMGs) it is a well proven fact that planar defects do exist, namely in form of shear bands (SBs) induced by plastic deformation. Consequently, the existence of planar defects in metallic glasses introduced by other means than deformation is possible. In this contribution, we present a detailed analysis of the structure, stability and topology of interfaces in nanoglasses by means of molecular dynamics computer simulations. We address the role of free volume, short-range order and thermal stability and study the mechanical properties of nanoglasses. Moreover, analogies of the properties of interfaces and shear-bands will be addressed.

MM 23.6 Tue 12:45 H 0107

Chemical disordering in intermetallic FeAl induced by cold rolling and folding — •Anna Findeisen[1,2], C. Gammer[1], C. Rentenberger[1], J. Eckert[2], and H.P. Karnthaler[1] — [1]University of Vienna, Physics of Nanostructured Materials, Wien, Austria — [2]Inst. of Complex Materials, IWF Dresden, Germany

Cold rolling and folding is used for the severe plastic deformation of the B2 ordered intermetallic compound FeAl. The structural changes induced by this deformation are studied by transmission electron microscopy (TEM) methods in combination with differential scanning calorimetry (DSC) and magnetic measurements. The TEM study re-

veals the formation of a nanocrystalline structure that is accompanied by a reduction of the long range order. The process of chemical disordering causes a transition from the initial paramagnetic state to a ferromagnetic one. DSC and magnetic measurements show that the reduction of order increases with increasing deformation. This leads to a state of saturation of strongly reduced chemical order that is formed by homogeneously distributed chemically ordered domains with a size of about 2 nm as revealed by TEM images. This structure containing a high density of defects is rather unstable as it starts to relax even at room temperature. The results of the transitions occurring upon heating of both the magnetic state and the process of re-ordering are compared with those of FeAl severely deformed by high pressure torsion [1,2,3]. [1] C. Mangler et al. Acta Mater. 58, 5631 (2010). [2] C. Mangler et al. J. Alloys and Comp. 509, Suppl. 1, 389 (2011) [3] C. Gammer et al. Scripta Mater. 65, 57 (2011).

MM 24: Functional Materials II

Time: Tuesday 11:30–12:30 Location: H 1029

MM 24.1 Tue 11:30 H 1029

Tunable optical bandgap of polymeric carbon nitride photocatalysts — •Christoph Merschjann, Tobias Tyborski, Steven Orthmann, Florent Yang, Martha Christina Lux-Steiner, and Thomas Schedel-Niedrig — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Polymeric carbon nitrides with the approximate sum formula C_3N_4 have been shown to be photocatalytically active for hydrogen production from water under visible light illumination. For an effective sunlight-driven process, the bandgap of the catalyst should be in the range of 2 eV.

We have investigated the optical bandgap of carbon nitride polymers synthesized at different temperatures between 400 °C and 610 °C. The bandgaps are found to be linearly decreasing in the given temperature range, parallel to a decrease of the lattice constants of the polymer network. Thus, a tunability is given in the range $2.5\,\mathrm{eV} < E_\mathrm{g}^\mathrm{dir} < 3.0\,\mathrm{eV}$. Possible reasons for the observed effects are discussed in the presentation.

MM 24.2 Tue 11:45 H 1029

First-principles study of La–H: structural change from LaH_2 towards LaH_3 — •Tobias C. Kerscher[1,3], Gunther Schöllhammer[1], Walter Wolf[2], Stefan Müller[3], Peter Herzig[1], and Raimund Podloucky[1] — [1]University of Vienna, Institute of Physical Chemistry, Vienna, Austria — [2]Materials Design s.a.r.l., Le Mans, France — [3]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Hamburg, Germany

By combination of first-principles density functional theory (DFT) and a cluster expansion (CE) with the UNCLE code [1], we investigate the interesting changes in the La–H system for the region between LaH_2 and LaH_3. These structural changes from the fluorite structure of the dihydride to the full trihydride drives a concentration-dependent metal-insulator transition ("switchable mirror") at $LaH_{\approx 2.8}$, as known by experiment. While our prior DFT study [2] had indeed already revealed the opening of a band gap at a hydrogen concentration close to LaH_3, we now show how a CE—based on input from DFT—predicts the structural changes in the full concentration range: It reveals the hydrogen's preference to occupy tetrahedral interstitial sites and the general formation of closely-paired hydrogen vacancies on octahedral interstitials. We compare our results to experiment.

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

[2] G. Schöllhammer *et al.*, J. Alloys Comp. **480**, 111–113 (2009)

MM 24.3 Tue 12:00 H 1029

Systematic Study of the Hydrogen-Sensing Performance of Buffered and Capped Pd and PdNi Layers for Plasmonic Applications — •Nikolai Strohfeldt, Andreas Tittl, and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, D-70569 Stuttgart, Germany

We present a systematic experimental study of the hydrogen-sensing performance of buffered and capped Pd and PdNi layers. We focus specifically on the aging behavior of the thin films and compare the magnitude of the sensor response as well as the response time for freshly evaporated and 4 and 11 day old samples.

We find an optimized sample geometry consisting of a PdNi layer capped with 3 nm Pt and buffered with 10 nm of CaF_2 that exhibits excellent signal stability and linear signal response in the concentration range from 0.5% to 5% hydrogen in nitrogen.

The samples were measured in a custom-designed sensor head consisting of a light emitting diode and two photo-diodes that allow us to simultaneously track the reflected and transmitted light from our samples.

The observed insights can be easily incorporated into plasmonic geometries to improve concepts like antenna enhanced or perfect absorber based hydrogen sensing and allow us to move one step closer to a durable and industrially feasible optical plasmonic hydrogen sensor.

MM 24.4 Tue 12:15 H 1029

Hybrid Simulation of Nucleation Grow under External Forces — Robert Glöckner[1], Christian Heiliger[2], and •Stefan Kolling[1,3] — [1]Deutsches Kunststoff-Institut, Abt. Mechanik und Simulation, Darmstadt, Germany — [2]Justus Liebig Universität Gießen, I. Physikalisches Institut, Gießen, Germany — [3]Technische Hochschule Mittelhessen, Institut für Mechanik und Materialforschung, Gießen, Germany

Polymer (Polypropylene) nucleation grow and morphology dynamics under external forces are simulated by using hybrid simulation techniques.

The ambient phase and its properties are simulated using finite element methods in order to to accomplish for external forces like stress / strain / steady fluid-flow.

Nucleation grow is implemented as user-defined material within the FEM-solver using cellular automata (CA) to describe nucleation grow statisticaly.

Percolation algorithms are used to analyze evolving morphology of the system and provide graph-theoretic techniques for caching intermediate integrating results of the CA's in order to auto-detect areas of similiar behaviour (automatic symmetry detection).

MM 25: Microstructure and Phase Transformations III

Time: Tuesday 11:45–13:00 Location: H 0106

MM 25.1 Tue 11:45 H 0106

Continuous freezing and delayering of argon in nanopores — •Klaus Schappert and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus Geb. E2.6, 66123 Saarbrücken, Germany

We investigate the freezing behavior of argon in nanoporous Vycor glass. The freezing temperature of substances adsorbed in nanopores is lowered in comparison to bulk. Bulk argon freezes at 84 K, whereas argon filled in Vycor glass seems to freeze only at about 75-76 K. However, the first few adsorbed layers of argon will not freeze at that temperature and remain in a liquid-like condition. We show that both the first and the second argon layer freeze continuously over a broad temperature range of at least 40 K. These layers completely freeze only far below the bulk freezing temperature, i.e. around 20 K. Whereas those two adsorbed layers remain stable during cooling, the third one becomes unstable around 66 K, rearranges, and solid capillary condensate is formed (delayering transition) [1].

[1] Klaus Schappert and Rolf Pelster, Phys. Rev. B 83, 184110 (2011)

MM 25.2 Tue 12:00 H 0106

Needle-like solutions in three-phase equilibrium binary alloys — •Guillaume Boussinot[1,2], Claas Hueter[1], and Efim Brener[2] — [1]MPIE, Duesseldorf, Germany — [2]PGI, Forschungszentrum Juelich, Germany

Three-phase equilibrium is a very common feature of phase diagrams of binary alloys. The phase transformations in the neighborhood of the corresponding equilibrium temperature are very diverse whether the system is eutectic, peritectic, monotectic... We give an overview of the two dimensional needle-like steady-state solutions in these systems, which are not described by the Ivantsov theory.

MM 25.3 Tue 12:15 H 0106

Martensitic phase transition of iron — •Bertrand Dupé[1,2], Bernard Amadon[1], Christophe Denoual[1], and Yves-Patrik Pellegrini[1] — [1]CEA, DAM, DIF, F-91297 Arpajon, France — [2]Institue of Theoretical Physics and Astronomy, University of Kiel, 24098 Kiel Germany

Even if Iron is a long studied element, several of its properties remain puzzling. One of them is the mechanism of martensitic phase transition from the bcc to hcp Phases. Even in the simplest description, a shuffle and a shear are involved in this transition [1]. Several authors have described the kinetic of the transition, using Minimum Energy Path calculations with ab initio calculations[2-4] with different physical assumptions for the coupling between shuffle and shear [3,4].

In this study, we propose a new path for the transition based on ab initio calculations. We discuss the path with respects to the NEB method. Our ab initio calculations also suggest that this transition might not involve a cooperative motion of atoms in contradiction to the common rule for martensitic transitions. The key role of magnetic ordering during the transition will be also adressed suggesting a more complex Ferromagnetic to Antiferromagnetic behaviour as previously seen [3,5].

[1] Burgers, W. G. Physica, 1934, 1, 561 [2]Ekman et al Phys. Rev. B, 1998, 58, 5296 [3] Johnson, D. F. & Carter, E. A. Journ. Chem. Phys., 2008, 128, 104703 [4] Liu, J. B. & Johnson, D. D. Phys. Rev. B, 2009, 79, 134113 [5] Friák, M. & Šob, M. Phys. Rev. B, 2008, 77, 174117

MM 25.4 Tue 12:30 H 0106

Role of carbon atoms on the transformation behavior in the high manganese steels — •Jaebok Seol[1], Changyung Park[2], Pyuckpa Choi[1], and Dierk Raabe[1] — [1]Max-Planck-Insititut für Eisenforschung, Dusseldorf, Germany — [2]Dept. of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Republic of Korea

In this study, we revealed that the γ into ϵ-martensitic transformation in Fe-17wt.% alloys was suppressed upon cooling by an increase in the carbon content by X-ray diffraction (XRD), electron back scattered diffraction (EBSD), and transmission electron microscopy (TEM). Also, the lattice parameter of austenite and the local distribution of stacking faults as a function of carbon composition have been observed through high resolution TEM. A direct observation method, based on a combined analysis of nano-secondary ion mass spectroscopy (nano-SIMS) and EBSD, was conducted to characterize the distribution of solute carbon in the alloys. Comparatively, atom probe tomography (APT) revealed that the inhomogeneous distribution of carbon played an important role on the austenite to ϵ-martensite transformation. Therefore, the segregation sites of carbon atoms in these steels were quantitatively elucidated.

MM 25.5 Tue 12:45 H 0106

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

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 microstructures can reduce strength and toughness of the material and are thus important to be studied. The intermediate stages of phase transformations in steels *during* the joining process can only be registered by *in situ* experiments. Therefore, *in situ* diffraction measurements using a transportable friction stir welding system ('FlexiStir') were performed at the HZG high-energy synchrotron beamlines HEMS and HARWI II at DESY. Additionally, the phase transformations occurring in the steels used for friction stir welding were studied using a dilatometer in the synchrotron beam. As a result, time resolved volume fractions of the steel phases during the phase transitions occurring during friction stir welding in different steels were obtained.

MM 26: Computational Materials Modelling V - Fracture and Other Failure Mechanisms

Time: Tuesday 12:00–13:00 Location: TC 006

MM 26.1 Tue 12:00 TC 006

First principles study of brittle cleavage processes in FeTi — •Li-Fang Zhu[1], Martin Friák[1], Antje Schlieter[2,3], Uta Kühn[2,3], Jürgen Eckert[2,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]IFW Dresden, Germany — [3]Dresden University of Technology, Dresden, Germany

Thorough understanding of atomistic mechanisms that are responsible for brittle failure of materials is crucial for many engineering applications. We employ density functional theory calculations to study the brittle cleavage under loading mode I in an important structural intermetallics, FeTi, along [100], [110], [111] and [211] directions. The calculated energy vs. separation curves are found to follow universal binding energy behavior (see e.g. [1]) and allow to determine the corresponding surface energies γ, cleavage energy G_b, and theoretical strength σ_b. Relations between cleavage and elastic properties are explored by applying the generalized Orowan-Gilman model [2]. Our study shows that the brittle loading along the [110] direction has the lowest strain to fail, as well as lowest cleavage energy and theoretical strength. These findings indicate that the preferred fracture occurs in single crystal FeTi along the (110) plane. We also find an onset of magnetism in FeTi when increasing the distance between the cleavage planes and show how it is responsible for termination-specific surface energy reductions.

[1] J. H. Rose, J. R. Smith, J. Ferrante, *Phys. Rev. B* **28** (1983) 1835.
[2] E. Orowan, *Rep. Prog. Phys.* **12** (1949) 185.

MM 26.2 Tue 12:15 TC 006

Atomistic simulations of grain boundary fracture in tungsten bicrystals — •Johannes J. Möller and Erik Bitzek — Lehrstuhl WW1: Allgemeine Werkstoffeigenschaften, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland

Brittle crack propagation in polycrystals frequently occurs along grain boundaries. Understanding the influence of grain boundary character (misorientation, interface plane, atomic structure) on the fracture behavior is therefore important for modeling fracture of polycrystalline materials. Although atomistic simulations are ideally suited to investigate the details of grain boundary fracture, relatively few systematic simulation studies exist.

Here we present results of atomistic fracture simulations in symmetrical low-Σ tilt grain boundaries in tungsten modeled by the Finnis-Sinclair potential. The fracture behavior (brittle crack advance, dislocation emission, twinning) and the critical stress intensity factors K_{Ic} were determined by molecular statics simulations.

Asymmetrically oriented slip systems lead to different fracture behavior in opposing crystallographic propagation directions. The simulations show that K_{Ic} for brittle fracture along grain boundaries can also dependent on the crack propagation direction and can be larger than the K_{Ic} for brittle fracture in single crystals of the corresponding orientation. The results are discussed in terms of thermodynamic and

kinetic aspects, and the concept of grain boundary trapping is introduced. Finally, consequences for mesoscopic models of grain boundary fracture are addressed.

MM 26.3 Tue 12:30 TC 006

Carbon at Σ5 STGB in molybdenum - from ab-initio results to traction-separation law — •Arshad Tahir, Rebecca Janisch, and Alexander Hartmaier — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany

Grain boundaries play an important role during plastic deformation and failure of poly-crystals. The presence of point defects, line defects or segregated second phase particles at the grain boundaries affect their mechanical properties, which in turn alter the hardness or fracture toughness of the poly-crystals favorably or adversely. In case of the bcc transition metals, which are the materials of interest for high temperature applications, grain boundaries and segregated impurities at grain boundaries play a vital role as well. Therefore, a sigma-5 (310)[001] Σ5 STGB present in molybdenum (Mo) has been atomistically investigated and the results are being used for fracture prediction at continuum scale.

The atomistic calculations were performed using the VASP employing GGA to DFT. After the initial convergence tests for the optimization of k-point meshing and energy cut-off of the plane wave basis set, a Σ5 (310)[001] STGB structure was constructed, relaxed and stable translation states along [310], [-130] and [001] were obtained. With this model uni-axial tests loaded perpendicular to the grain boundary plane having different C contents were performed. From these results, traction separation data has been derived that is being used for the parameterization of cohesive zone model to predict fracture of Mo bicrystals at continuum level using finite element analysis.

MM 26.4 Tue 12:45 TC 006

Ab-initio Study on Liquid Metal Embrittlement in the Fe/Zn System — •Klaus-Dieter Bauer[1], Mira Todorova[2], Kurt Hingerl[1], and Jörg Neugebauer[2] — [1]Center for Surface and Nanoanalytics, Johannes Kepler University Linz, Austria — [2]Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

In the manufacturing of high quality steels products, processing steps and costs can be saved by hot-forming (already) coated steel plates. For galvanized sheets however, a degradation of workpieces' quality is observed, caused by *Liquid Metal Embrittlement* (LME) of the steel bulk coming in contact with the liquid zinc phase. To get insight into the mechanism of LME in the Fe/Zn system we perform density-functional-theory calculations, considering the [111]Σ3 and [110]Σ5 tilt grain boundaries in bcc iron (ferrite). Investigating the applicability of the Griffith model, we compare the interface energies of the grain boundaries and associated surfaces for different Zn coverages. Our results show Zn wetting to stabilize the grain boundaries, and even stronger the associated surfaces, yet not sufficiently to cause spontaneous surface formation. This is compatible with the outcome of experiments performed at Voestalpine AG.

MM 27: HV Curtin

Time: Wednesday 9:30–10:00 Location: TC 006

Invited Talk MM 27.1 Wed 9:30 TC 006

First-principles Predictions of Solute Strengthening in Al and Mg alloys — •William Curtin[1] and Gerard Leyson[2] — [1]Ecole Polytechnique Federale de Lausanne — [2]Brown University

A quantitative, parameter free model to predict the flow stress as a function of temperature and strain rate of such alloys is presented. The model builds on analytic concepts developed by Labusch but introduces key innovations rectifying shortcomings of previous models. To accurately describe the solute/dislocation interaction energies in and around the dislocation core, density functional theory and a flexible-boundary-condition method are used. The model then predicts the zero temperature flow stress, the energy barrier for dislocation motion, and thus the finite temperature flow stress. Predictions of the model are in excellent agreement for a range of Al alloys and basal strengthening in Mg-Al as a function of solute concentration and temperature. This success demonstrates that computational materials science can provide quantitative guidance to materials design for properties controlled by complex interactions of defects, in this case flow stress controlled by dislocation interactions with solutes.

MM 28: Topical Session Theory meets Experiment I - Intermetallics and Steels

Time: Wednesday 10:15–11:30 Location: TC 006

Topical Talk MM 28.1 Wed 10:15 TC 006

Some Contributions to Materials Design from Combined Three Dimensional Observation of Materials by Atom Probe Tomography and Three Dimensional Atomistic Modelling — •George Smith — Department of Materials, Oxford University, Parks Road, Oxford OX1 3PH, United Kingdom

Two exciting new developments have come together in recent years in the field of materials science. For the first time, we are able to observe experimentally the three-dimensional atomic-scale chemistry of solids, by atom probe tomography. Also, we are now able to carry out large-scale computer modelling of materials in three dimensions at the atomic level. The combination of experiment and theory opens totally new horizons for intelligent materials design and development. Three case studies, from very different fields, will be presented to illustrate the power of this new approach. The first relates to the development of improved pressure vessel steels for energy generation. The second involves the improvement of manufacturing methods for magnetic sensors for use in computer memories. And the third demonstrates the use of atomic-scale imaging and analysis to assist in optimising the activity of core-shell nanoparticle catalysts for fuel cell applications.

MM 28.2 Wed 10:45 TC 006

Decomposition of cementite under strain in pearlitic steels: An ab intio study — •Gholamali Nematollahi, Johann von Pezold, Jörg Neugebauer, and Dierk Raabe — Max-Planck Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Severely plastically deformed pearlitic wires are amongst the strongest materials known to mankind. Despite extensive research the fundamental mechanisms underlying the extraordinary strength of this α-Fe/Fe3C composite are still unclear. Experimental evidence suggests that the applied strain induces a substantial migration of C atoms from cementite lamellae into adjacent ferrite particles, resulting in a dramatically increased C concentration in the ferrite matrix after the plastic deformation (by ~ 9 orders of magnitude). We therefore consider here the stability of C interstitials in ferrite and of C vacancies in cementite as a function of the relevant strain state, using density functional theory. Our analysis reveals a substantial strain-induced stabilization of the C interstitial in ferrite and a minor destabilization of the C vacancy in cementite. Using this insight we are able to explain the experimentally observed partial dissolution of cementite in severely plastically deformed pearlitic wires by the strain-induced stabilization of C interstitials in ferrite.

Keywords: Density functional theory, Ferrite, Cementite, Carbon interstitial, vacancy formation energy

MM 28.3 Wed 11:00 TC 006

On the dependence of elastic properties on the point-defect content in vacancy-rich β-NiAl — •Sascha B. Maisel and Stefan Müller — Insitute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

The high-temperature alloy β-NiAl can tolerate an exceptionally high number of point defects in the form of vacancies or anti-site atoms. In fact, the B2 phase which $Ni_{50}Al_{50}$ prominently exhibits is still stable

up to vacancy-rich crystals with a stochiometry of around $Ni_{42.5}Al_{50}$ [Warlimont77]. However, we find that many assumptions that are commonly used when describing the dependence of elastic constants on point defects in single crystals do not hold for β-NiAl. In particular, the Wagner-Schottky approximation is not valid and common analytical descriptions [Pistorius70] fail due to cell volume changes at high vacancy contents. Moreover, the widely used five parameter extrapolation [Warlimont77] for the elastic moduli in β-NiAl is not correct for very high defect concentrations. We present improved values for the elastic behavior in the high-vacancy regime derived from fully relaxed first-principles structures.

References:
N. Rusovic, H. Warlimont: Phys. Stat. Sol. 44, 609 (1977)
M. Pistorius: Z. angew. Phys. Z9, 145 (1970)

MM 28.4 Wed 11:15 TC 006

Understanding H-induced failure mechanisms in metallic alloys: The role of attractive H-H interactions in nano-precipitate formation — •Johann von Pezold, Alexander Udyansky, and Joerg Neugebauer — Max Planck Institut fuer Eisenforschung GmbH, Duesseldorf

Attractive H-H interactions have recently been shown to induce the formation of local hydride precipitates even in non-hydride forming matrices, such as Ni [1]. The formation of these nano-hydrides in the strain field of lattice defects such as crack tips and dislocations has been correlated to the long-standing problem of hydrogen embrittlement in these metals. In this study we systematically investigate H-H interactions in a range of fcc matrices, including Ca, Mn, Fe, Co, Ni, Al and Pd, using density functional theory. While the interaction between H atoms in first nearest neighbour interstitial sites is generally attractive, the nature of this interaction is strongly system and site dependent. Hence, the interaction between octahedral sites is predominantly of elastic nature, while interactions between tetrahedral sites exhibit a significant chemical contribution. Based on this study the formation of nano-hydrides in fcc metals will be critically discussed.

[1] J. von Pezold, L. Lymperakis and J. Neugebauer, Acta Mat. 59, 2969 (2011).

MM 29: Topical Session Bulk Nanostrucured Materials VI - Mechanical Properties I

Time: Wednesday 10:15–11:45 Location: H 0107

Topical Talk MM 29.1 Wed 10:15 H 0107

Texture, microstructure and mechanical properties of ARB aluminium laminates — •Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany

Aluminium sheets with layers of different purity (A: 99.999 and B: 99.5) produced by accumulative roll bonding (ARB) were studied for different numbers of ARB cycles. Both material layers show a contrasting dynamic recrystallization behaviour with A and B recrystallizing discontinuously and continuously, respectively. The layered structure is stable up to 6 cycles, for higher cycles slightly necking starts. Global textures were measured by neutron diffraction while local textures of the different layers were measured by X-ray as well as electron backscatter diffraction (EBSD). The microstructure is analyzed from EBSD mappings. The mechanism of texture and microstructure development will be discussed in detail through thickness and with the number of ARB cycles. The strength and Lankford parameter were 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 simulations on the plastic anisotropy of laminated structures.

MM 29.2 Wed 10:45 H 0107

Mechanical properties of Ti- and TiAl3 reinforced ultrafine-grained aluminium — •Christian Werner Schmidt, Heinz Werner Höppel, and Mathias Göken — Institute I: General Materials Properties, Department Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg

In this work titanium particles (d ~ 2 to 4 micron) are introduced in a highly controlled manner by airgun spraying from aqueous suspension into aluminium AA1050A by accumulative roll bonding (ARB). A layered ultrafine-grained (UFG) material with extraordinary mechanical properties, further reinforced with metallic particles is produced. By diffusional annealing, the metallic titanium particles are converted to the very hard intermetallic phase TiAl3, where the UFG matrix is recrystallized and softened. In order to re-establish the UFG structure three subsequent ARB cycles are executed. By tensile testing of the different states, strengthening effects by the grain size, particle volume fraction, and material are distinguished. Therewith the basic understanding of the mechanism of reinforcement by particles in ultrafine-grained metals is enhanced. The TiAl3 reinforced ultrafine-grained aluminium sheets are very promising due to enhanced strength as well as clearly improved thermal stability of the UFG structure caused by particle reinforcement.

MM 29.3 Wed 11:00 H 0107

Grain boundary mediated plasticity in nanocrystalline metals and their alloys: On the interplay of mesoscopic sliding, coupled motion and segregating solutes — •Jonathan Schäfer and Karsten Albe — TU Darmstadt, Darmstadt, Germany

As the grain size is decreased into the lower nanometer (nm) range, the contribution of grain boundary (GB) mediated processes to low temperature plastic deformation increases. Hahn and Padmanabhan postulated that in nanocrystalline materials neighboring GBs can align themselves, allowing for GB sliding on a mesoscopic scale. Depending on the misorientation of the boundary, it was shown by Cahn et al., that GB motion can couple to shear deformation and move perpendicular to the shearing direction (out of the shear plane). This leads to a competition between mesoscopic GB sliding and coupled GB motion. For studying this competition and the effect of segregating solutes, we utilize molecular dynamics simulations, where nc Cu and CuNb serve as model systems. By testing a suitable microstructure under tensile and compressive load, we find that depending on the type of the GB, coupled motion out of the sliding plane is observed. This inevitably hinders any potential alignment and therefore prohibits mesoscopic GB sliding. For the case of samples with segregating solutes in the GB we show that it is a delicate function of composition, whether a given GB is pinned in place allowing for mesoscopic sliding or can leave the slide plane by coupled GB motion.

MM 29.4 Wed 11:15 H 0107

Thermal stability and strain-rate sensitivity of nanocrystalline Ni and a Ni/Al2O3 nanocomposite — •Michaela Prell[1], Karsten Durst[1], Harald Natter[2], Anne Jung[2], and Mathias Goeken[1] — [1]Institute of General Materials Properties, Department of Materials Science and Engineering, University of Erlangen-Nürnberg — [2]Physical Chemistry, Saarland University, Saarbruecken, Germany

The thermal stability and strain-rate sensitivity of a nickel-alumina nanocomposite and nanocrystalline Ni with different amount of grain refiner has been studied using compression tests up to 300°C and microstructural investigations with scanning and transmission electron microscopy. It is found that during deposition, the Al2O3 particles form clusters, which are evenly distributed in the nc-Ni microstructure. The initial hardness and flow stress of the nc-Ni/Al2O3 is smaller compared to nc-Ni, but with heat treatment or testing at higher temperatures, nc-Ni/Al2O3 shows a higher strength and higher strain rate sensitivity. For nc-Ni, even at an annealing temperature of 250°C strong grain coarsening has been found, where initially large grains are embedded in a nanocrystalline matrix. For longer annealing times, a stable ultrafine grain size of ~1 micron was observed. During compression test at 250°C however, homogenuous grain coarsening is observed. The stability of the microstructure against coarsening due to the Al2O3 particles is discussed as one of the main reasons for the enhanced properties of the nanocomposite.

MM 29.5 Wed 11:30 H 0107

Effects of alloying and temperature on the mechanical behavior of nanocrystalline Palladium alloys — •Ruth Schwaiger, Thomas Neithardt, and Oliver Kraft — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM)

Over the past decade significant advances in understanding the deformation mechanisms in fine-grained metals and alloys have been made. It is now well accepted that in the grain size regime up to about 50 nm the dislocation activity is significantly reduced. Other deformation mechanisms such as nucleation and motion of partial dislocations, grain boundary sliding or grain rotation and grain boundary motion were shown to gain importance, which is corroborated by the small activation volumes and increased strain rate sensitivity typically observed in nanocrystalline metals. In our work, we investigated nanocrystalline Pd und PdAu-alloys using strain rate sensitive indentation and microcompression testing. In order to better understand the deformation mechanisms and their thermal activation, the experiments were conducted at different temperatures ranging from 10°C to 90°C. In this temperature range, no microstructural changes were observed. While the hardness was observed to increase with increasing alloying content, no significant alloying effect on the strain rate sensitivity and activation volume was observed at room temperature. For low alloying concentrations, the strain rate sensitivity and the apparent activation volume were observed to change with temperature.

MM 30: Functional Materials III

Time: Wednesday 10:15–11:30 Location: H 0106

MM 30.1 Wed 10:15 H 0106

Impact of alloying elements on H solubility in steels — •Roman Nazarov, Tilmann Hickel, and Jörg Neugebauer — Max Planck Institute für Eisenforschung, Duesseldorf, Germany

Hydrogen embrittlement is a major failure mechanism in modern high-strength steels. Recent experimental studies indicate that alloying steels with selected elements largely improves their resistivity with respect to this failure mechanism. The origin of this mechanism, however, is unknown. We have therefore studied how various alloying elements affect H trapping in different steel phases. The solution enthalpies for a large set of common alloying elements in these phases have been calculated. Our results show that substitutional elements (Al, Cr, Mo, Nb, Si, Ti) energetically prefer the ferrite phase, while interstitial elements (B, C, and N) prefer austenite. Computing the interaction of these alloying elements with H we find that in the ferrite phase most of them repel an H atom from their neighborhood. In an austenitic matrix Nb and Ti bind H atoms in the first shell. Furthermore, these elements expand the Fe matrix, resulting in an increased interstitial volume and subsequent increased H solubility. In contrast, in an austenitic matrix P, Si and S repel H from their neighborhood. Based on this insight we derive a thermodynamic model which allows us to determine the solubility of H in real steels at any given temperature and H chemical potential.

MM 30.2 Wed 10:30 H 0106

Scale Bridging Modeling of Hydrogen Embrittlement — •Dominique Korbmacher, Claas Hüter, Johann von Pezold, and Robert Spatschek — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen is known to embrittle many metals and steels, resulting in the premature failure of these materials. As a prototype of such a material we investigate nickel, which does not form hydrides under standard conditions of temperature and pressure. However, the attractive hydrogen-hydrogen interactions within the metal matrix have been shown to induce the formation of nano-hydrides in distorted regions of the lattice (crack tips or dislocations) even at only moderately enhanced hydrogen chemical potentials. We perform atomistic Monte-Carlo simulations to investigate the formation of the hydride phase as a function of the hydrogen chemical potential and use these data to parametrise a thermodynamic model with special attention to the role of elastic effects, which drastically influence the behavior in the two-phase region. The results of this analysis are then used in mesoscale simulations for the formation of hydride zones around crack tips. To this end we simulate the diffusive flux of hydrogen towards the tensile regions of a crack, and investigate the growth of the hydride zone and its steady state size depending on the stress intensity factor and the hydrogen supply. The results are in agreement with analytical scaling relations.

MM 30.3 Wed 10:45 H 0106

Intrinsic point defects in ZnSb — Lasse Bjerg[1], •Georg K. H. Madsen[2], and Bo B. Iversen[1] — [1]Department of Chemistry & iNANO, Aarhus University, Denmark — [2]Department of Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Germany

Several efficient thermoelectric materials have been found among the ternary Zintl antimonides. If the band structure is highly asymmetric around the band gap, the efficiency as either n- or p-type may differ significantly. The Zintl antimonides have generally been found to be p-type. Surprising this also holds true for the narrow band gap binary ZnSb and Zn_4Sb_3.

Using ab initio calculations we investigate intrinsic point defects in ZnSb as a possible origin of the p-type conductivity. Negatively charged Zn vacancies are found to have a low formation energy, leading to an intrinsic p-type behavior. We discuss this finding as a general explanation of p-type conductivity in Zintl antimonides and how to overcome the doping limits in these materials.

MM 30.4 Wed 11:00 H 0106

Combined Nuclear Magnetic Resonance and x-ray diffraction study on single crystalline LiMnPO4 — •Christian Rudisch, Sven Partzsch, Jochen Geck, Hans-Joachim Grafe, and Bernd Büchner — IFW Dresden

LiMnPO4 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 as well as the effect of disorder on the mobility in this material is not well understood. The advantage of the use of single crystals is that the NMR 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 interstitial 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. We present results of a combined NMR and X-ray diffraction study which indicate a substantial degree of disorder in LiMnPO4, where the Li ions are distributed along the b- and c-axis of the crystal. The type of disorder underlines theoretical calculations which claim a possible Li-mobility in b direction. The impact of disorder on the Li mobility will be discussed.

MM 30.5 Wed 11:15 H 0106

Ultra Fast and Anisotropic Diffusion of Lithium in Silicon Nanostructures — •Stefan Wagesreither, Alois Lugstein, and Emmerich Bertagnolli — Institute for Solid State Electronics, TU-Wien, Vienna, Austria

Silicon based anodes could improve the lithium ion battery technology with a theoretical tenfold higher capacity in comparison to commercially used graphite anodes. Besides the capacity, fast charge and discharge rates and the closely associated diffusion velocity are important aspects of the battery. By improving the diffusion of lithium in silicon, an performance increase of novel silicon anodes for lithium ion batteries could be achieved. Therefore the dependency of lithium diffusion on the crystallographic directions of silicon was investigated with regard to the diffusion velocity. The lithiation of submicron silicon beams isolated on SiO_2 showed an anisotropic behavior with a dependency on the beam direction along the (100) plane. In silicon beams with <110> direction the lithiation was more prolonged than in <100> beams. With an approximation of the Einstein relation $L = \sqrt{(D \cdot t)}$, a diffusion coefficient of $D(50°C) = 3.36 \cdot 10^{-7} cm^2/s$ was calculated which is 5 orders of magnitude higher than results for bulk silicon at the same temperature. This result is reflected in the formation of lithium silicide dendrites in the favored <110> direction after contact of lithium with a silicon thin film at room temperature.

MM 31: Nanocharacterization

Time: Wednesday 10:15–12:15 Location: H 1029

MM 31.1 Wed 10:15 H 1029

HR(S)TEM and TAP analyses of embedded Pb nanoparticles — •Anna Moros, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

In the present work nanoscaled Pb particles embedded in an Al(Ga) matrix with 3 at.% Ga were processed by melt spinning. Using the ChemiSTEM technology integrated into a FEI Tecnai Osiris 200 kV microscope, elemental mappings have been performed and revealed Ga segregation at grain boundaries. This is a well known process (grain boundary poisoning) leading to an intergranular embrittlement of the Al matrix. However, Ga segregation also occurred at the nanoscaled embedded Pb particles. In order to investigate the particle-matrix interface precisely, high resolution micrographs were taken at the JEOL JEM-ARM 200F. Geometric phase analysis has been used to evaluate the strain state of the heterogeneous particle-matrix interface. It is shown, that the lattice parameter mismatch between the Pb particle and the Al(Ga) matrix is reduced in comparison with the AlPb composite. In order to verify whether the Ga is alloying with Pb or not, Tomographic Atom Probe (TAP) was used. These experimental results are presented and critically discussed. Funding by DFG is gratefully acknowledged.

MM 31.2 Wed 10:30 H 1029

Characterization of nano-particle size and orientation using auto-correlation analysis of electron microscopy images — •Thomas Weiss, Dieter Akemeier, and Andreas Hütten — Universität Bielefeld, 33615 Bielefeld, Germany

The determination of the size, in particular the size-distribution, of nano-particles has been carried out so far by counting each particle. This method is time consuming, whence an automated method is desired to avoid this procedure.

Images of nano-particles taken by electron microscopy are analysed by auto-correlation analysis. Using auto-correlation analysis it allows one to determine the concentration of the particles, the size-distribution and, if existent, the oriented alignment. In order to compare these results nano-particles on an image plane are simulated, where the further analysis has been made by auto-correlation.

This method can be applied to images of any kind, for example of nano-particles observed in electron microscopy or cross sections of magnetic beads.

MM 31.3 Wed 10:45 H 1029

Iron L- and M-edges of iron containing minerals measured by inelastic x-ray scattering — •Alexander Nyrow[1], Christian Sternemann[1], Max Wilke[2], Christoph Sahle[1], Kolja Mende[1], Laura Simonelli[3], Robert Gordon[4], Nozomu Hiraoka[5], Florian Wieland[1], Metin Tolan[1], and John Tse[6] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Deutsches GeoForschungsZentrum, Section 3.3, Potsdam, Germany — [3]European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France — [4]PNC-SRF, Dept. of Physics, Simon Fraser University, Burnaby, BC, Canada — [5]National Synchrotron Radiation Research Center, Taiwan — [6]University of Saskatchewan, Department of Physics and Engineering Physics, Saskatoon, Canada

Iron is one of the most important elements which form the Earth's mantle. Most physical properties of the Earth's interior have been extracted from seismological observations or structural laboratory studies of phases attendant in the Earth's body. Depending on pressure, temperature and oxygen fugacity the Fe^{2+}/Fe^{3+} ratios and the Fe spin-state of iron-bearing minerals can vary significantly. Thus, a quantitative determination of the oxidation state of iron is crucial for the understanding of the thermodynamic properties of these minerals at the conditions of the deep Earth. In this study Fe $L_{2/3}$ and $M_{2/3}$-edges of different iron oxides and iron containing minerals measured by x-ray Raman scattering are presented in comparison with results of soft x-ray absorption and electron energy loss spectroscopy. Furthermore, the momentum transfer dependency of the Fe $M_{2/3}$-edge is discussed.

MM 31.4 Wed 11:00 H 1029

X-ray Raman scattering: A spectroscopic tool to study low Z elements at extreme pressure and temperature — •Kolja Mende[1], Alexander Nyrow[1], Christian Sternemann[1], Christian Schmidt[2], Max Wilke[2], Christoph J. Sahle[1], Thorsten Brenner[1], Laura Simonelli[3], Marco Moretti Sala[3], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, TU Dortmund, Dortmund, Germany — [2]Geoforschungszentrum Potsdam, Potsdam, Germany — [3]European Synchrotron Radioation Facility, Grenoble, France

In situ studies of materials under conditions of geological relevance, i.e. high pressure and high temperature, can only be performed using diamond anvil cells in combination with resistive or laser heating. Due to highly absorbing sample environments, the study of absorption edges for binding energies between 10 eV and 2 keV of low and intermediate Z elements such as sodium, aluminum, silicon, etc. is hardly possible using electron or soft x-ray spectroscopy. Here, x-ray Raman scattering (XRS), an energy loss spectroscopy using hard x-rays as a probe, provides a unique experimental method. XRS yields similar information as soft x-ray absorption and electron energy loss spectroscopy. It is very sensitive to changes of the electronic and local atomic structure and allows to probe different excitation channels by variation of the momentum transfer. With this method, the partial unoccupied density of states can be determined. The capabilities of this experimental technique for geophysical applications are discussed for selected examples.

MM 31.5 Wed 11:15 H 1029

Probing intermediate valence in rare-earth compounds by X-ray excitations goes along with significant final state effects — •K. Kummer[1], Yu. Kucherenko[2], S. Danzenbächer[2], C. Krellner[3], C. Geibel[3], S. L. Molodtsov[4], C. Laubschat[2], and D. V. Vyalikh[2] — [1]ESRF, Grenoble, France — [2]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — [4]European XFEL GmbH, Hamburg, Germany

Interaction with itinerant valence states can cause an instability of the 4f shell in rare-earth intermetallics. The resulting intermediate valence of the rare-earth ions often depends on applied pressure, temperature or chemical doping and is closely related to the magnetic and transport properties of the material. X-ray spectroscopies like 4f photoemission, X-ray absorption, or resonant inelastic X-ray scattering are very sensitive to different 4f configurations and have thus become a standard tool to study intermediate valent behavior. However, comparing results of the different X-ray spectroscopic techniques among each other and with numbers obtained with low-energy excitation methods one often finds discrepancies larger than the accuracy of each of the employed techniques. We performed theoretical simulations which reveal that final state effects lead to non-linear relations between the the weight of a 4f configuration in the ground state and its spectral weight. Valence determination from X-ray spectroscopic data requires a quantitative characterization of those final state effects which we demonstrate here at the example of intermediate valent Yb compounds.

MM 31.6 Wed 11:30 H 1029

Structural investigations on the interfacial layer between diamonds and metal matrices in diamond tools via X-ray scattering — •Andre Steffen[1], Michael Paulus[1], Christian Sternemann[1], Manuel Pinho Ferreira[2], Christian Kronholz[2,4], Ralph Wagner[3], Wolfgang Tillmann[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, D-44221 Dortmund — [2]Institute of Materials Engineering, TU Dortmund, D-44221 Dortmund — [3]Fachbereich C - Abteilung Physik, Bergische Universität Wuppertal, D-42097 Wuppertal — [4]Benteler Tube Management GmbH, D-33104 Paderborn

Diamond grinding tools have widely established its usage in machining and cutting of hard materials such as natural stone and concrete. These diamond metal composites are mainly fabricated powdermetallurgically. The sintered metal serves as a boundary matrix for the embedded diamond grains. Therefore the bonding type of the diamonds in the metal matrices is of essential relevance. So it is of important interest if the interfacial area between the diamonds and metal matrices consist of metal-carbides, solid solutions of carbon in metal or even graphite. In this work diamond metal (Co, Fe, Cr) composites have been investigated by X-ray absorption near-edge fine structure spectroscopy (XANES) and X-ray diffraction (XRD) in order to anal-

yse the structure of the interfacial layer between the diamonds and the metal matrices. First analysis of the XANES data indicate changes in the local structure due to the sintering process. XRD studies show the formation of graphite.

MM 31.7 Wed 11:45 H 1029

Material Processing with Femtosecond Laser Pulses — •Steffen Fiedler, Robert Irsig, Anna Oniszczuk, Josef Tiggesbäumker, Conrad Schuster, Anna Svanidze, Neeke Rothe, Stefan Lochbrunner, and Karl-Heinz Meiwes-Broer — Institute of Physics, University of Rostock, Germany

Material modifications on the μm-scale are required in many applications, e. g. in micromechanics or modern medical implant technologies. Pulsed laser light sources are powerful tools dedicated to replace conventional methods of mechanical processing in many cases.

In laser machining the working area is confined to the laser focus with minimal effects on the functionality of the surrounding surface. Even higher precision becomes available for ultrashort femtosecond laser pulses by a reduction of heat transfer into the material due to the short interaction time [1]. Furthermore the high intensity of femtosecond laser pulses leads to a different ablation mechanism that in principle allows for processing arbitrary materials. In order to achieve this it is necessary to adapt the laser parameters for each sample. Especially when applying shaped laser pulses an improved precision is accessible [2].

The goal of this project is to optimize the working conditions and the quality of the machining process for different specimens and their implementation in medical applications in particular.

[1] B. N. Chichkov et al., Appl. Phys. A 63, 109 (1996)

[2] L. Englert et al., Appl. Phys. A 92, 749 (2008)

MM 31.8 Wed 12:00 H 1029

Mechanism of nanostructure formation during in in-situ consolidation of mechanically-milled copper — •Mohsen Samadi Khoshkhoo[1,2], S. Scudino[1], H. Bahmanpour[3], A. Kauffmann[1], J. Freudenberger[1], R. Scattergood[3], M. J. Zehetbauer[4], C. C. Koch[3], and J. Eckert[1,2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institut für Werkstoffwissenschaft, D-01062 Dresden, Germany — [3]Department of Materials Science and Engineering, North Carolina State University, Campus Box 7907, Raleigh, NC 27695-7907, USA — [4]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria

Bulk nanocrystalline Cu samples have been produced by in-situ consolidation during mechanical milling. The effect of milling temperature and milling intensity on the structure of the samples was studied in detail and particular attention was paid to reach the optimal conditions for successful in-situ consolidation. Microstructural evolution during milling was monitored using X-ray diffraction analysis assisted with the whole powder pattern modeling (WPPM) technique. The results show that the dislocation density increases continuously with milling time, reaches a maximum and then decreases with further milling. Transmission electron microscopy (TEM) investigations carried out before and after the observed maximum of dislocation density reveal that dynamic recrystallization is responsible for the reduction of dislocation density. The mechanism of nanostructure formation through dynamic recrystallization was studied in detail using high-resolution TEM analysis and scanning electron microscopy.

MM 32: Functional Materials IV

Time: Wednesday 11:30–12:30 Location: H 0106

MM 32.1 Wed 11:30 H 0106

Studying the lithium deintercalation in thin $LiCoO_2$ films by electro-chromatic measurements — •Tobias Stockhoff, Tobias Gallasch, Frank Berkemeier, and Guido Schmitz — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Münster (Westf.), Germany

$LiCoO_2$ powder is one of the important components of today's lithium ion battery technology. In this work, we investigate thin $LiCoO_2$ films with respect to the intercalation/deintercalation of lithium ions, for potential application in all solid-state thin film batteries. For this purpose, $LiCoO_2$ films between 5 and 400 nm in thickness, were deposited onto ITO-coated glass substrates by rf-ion beam sputtering. The structure and stoichiometry of the films was checked by means of transmission electron microscopy (TEM), while basic electrochemical properties of the layers were studied by chrono-amperometry, cyclic voltammetry (CV), and galvanostatic intermittent titration technique (GITT).

Additionally, the reversible intercalation and deintercalation of lithium is demonstrated by measuring the optical transmission through the thin film system, since the colour of the $LiCoO_2$ films strongly depends on their lithium concentration. Using this electro-chromatic effect, the diffusion coefficient of lithium inside the films is determined, and the local lateral distribution of lithium is studied in-situ, using optical microscopy.

MM 32.2 Wed 11:45 H 0106

TEM on electrochemically cycled thin film electrodes — •Tobias Gallasch, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhlems-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Thin film electrodes (150 nm) of well known Li intercalation materials, such as $LiCoO_2$ and V_2O_5 are prepared by ion beam sputtering. XRD, analytical TEM (TEM/EELS) and conductivity measurements were employed to carefully optimize the sputter parameters. The functional efficiency of the thin films as battery material was verified in detailed Cyclic Voltammetry and Chrono-Potentiometry studies. In the case of V_2O_5 thin films high capacities (300 mAh/g after 25 voltammetric cycles) and high cycling stabilities (250 mAh/g at constant current, 1C) are found which are in the range of the theoretical capacity (400 mAh/g).

In contrast to conventional capacity studies at bulk material, we provide a model system with defined geometry which allows investigating fundamental Li transport and electrode aging processes on smallest length scales. Special focus is therefore dedicated to electron energy loss-spectroscopy (EELS) which is demonstrated to be sensitive to even minor changes in composition. V_2O_5 thin films show a crystalline to amorphous transition during cycling which is studied in detail by analytical and high resolution TEM. The goal of this work is the combination of both, electrochemical and structural data to obtain information about Li transport mechanisms which are of fundamental interest in this field.

MM 32.3 Wed 12:00 H 0106

Synthesis of metastable transition metal compounds for electrochemical energystorage — •Carsten Jähne[1], Christoph Neef[1], Hans-Peter Meyer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg — [2]Institut für Geowissenschaften, Universität Heidelberg, INF 236, 69120 Heidelberg

Advanced cathode materials for Lithium-Ion batteries are currently under intense research. We apply microwave-assisted hydrothermal reactions which enable synthesizing materials with a huge variety of morphologies and with grains down to the nanoscale. Here we report on the synthesis of two metastable materials LT-$LiCoO_2$ and non-olivine $LiCoPO_4$. We note that the latter exhibits a theoretically predicted crystal structure not observed yet in experiment. Crystal structure, morphology and Co-valancies were determined by means of XRD, SEM and magnetisation studies, respectively. The thermal stability of $LiCoPO_4$ was investigated with DSC/TGA. The electrochemical behaviour of both materials was analyzed by cyclic voltammetry (CV) and charge-discharge-cycling (GITT).

MM 32.4 Wed 12:15 H 0106

Aerographite: A new carbon nanomaterial with densities below 0.2 mg/ccm and outstanding mechanical properties — •Arnim Schuchardt[1], Matthias Mecklenburg[2], Yogendra Kumar Mishra[1], Sören Kaps[1], Rainer Adelung[1], Andriy Lotnyk[3], Lorenz Kienle[3], and Karl Schulte[2] — [1]Institute for Materials Science, Functional Nanomaterials, University of Kiel, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Institute of Polymers and Composites, Hamburg University of Technology, Denickestr. 15,D- 21073 Ham-

burg, Germany — [3]Institute for Materials Science, Synthesis and Real Structure, University of Kiel, Kaiserstr. 2, D-24143 Kiel, Germany

Energy storage application like batteries or supercapacitors call for new carbon electrode materials which can be designed with respect to the requirements of the individual application. We will present our work about a new Carbon nanomaterial called Aerographite which has the lowest density of all materials yet known (density < 0.2 mg/ccm) but is still mechanically robust and highly flexible. The foam like hierarchical 3D network structure has been investigated by various methods like SEM, TEM, XRD and EELS and based on the results a growth model was developed. It will be reported about the synthesis of Aerographite and its potential to design the material in the desired manner for the individual application. Further on, measurements regarding the electrical conductivity and the mechanical tensile/compression behaviour will be discussed. Experimental results of an Aerographite electrical double layer capacitor will be elaborated in more detail.

MM 33: Topical Session Theory meets Experiment II - Nanocomposites and Microstructure

Time: Wednesday 11:30–13:00 Location: TC 006

Topical Talk MM 33.1 Wed 11:30 TC 006

Correction of spherical and chromatic aberration: towards the ultimate performance in transmission electron microscopy — •Joachim Mayer — Central Facility for Electron Microscopy, RWTH Aachen University, 52074 Aachen and Ernst Ruska-Centre, Forschungszentrum Jülich, 52425 Jülich

The introduction of aberration correctors has revolutionized the development of TEM and STEM instrumentation. Only shortly after the development and installation of the first TEM with a corrector for the spherical aberration [1], commercial instruments with aberration correctors are now offered by all major manufacturers. In order to provide a platform for these novel developments and based on the experience with the first aberration corrected TEM [2], Research Centre Juelich and RWTH Aachen University have jointly founded the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C). With the recent installation of PICO, the second high resolution TEM in the world which is equipped with a corrector for the chromatic aberration, a broad range of new methods is now available. Research at the Ernst Ruska-Centre focuses on the development of new quantitative methods in TEM and on their application in materials science and solid state physics [3]. The most important fields of application are nanoelectronics and nanomaterials for energy-related systems. [1] M. Haider, H. Rose, S. Uhlemann, E. Schwan, B. Kabius, and K. Urban, Nature 392 (1998) 768. [2] C.L. Jia, M. Lentzen, and K. Urban, Science 299 (2003) 870. [3] C. L. Jia, S. B. Mi, K. Urban, I. Vrejoiu, M. Alexe, D. Hesse, Nat. Mater. 7 (2008) 57.

MM 33.2 Wed 12:00 TC 006

Atomic modeling of asymmetric tilt grain boundaries in Al_2O_3 — •Haksung Lee[1], Paul Tangney[2], Matthew Foulkes[1], and Michael Finnis[1,2] — [1]Department of Physics, Imperial College London, Exhibition Road, London SW7 2AZ, UK — [2]Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, UK

The atomic level characterization of grain boundaries is a fundamental subject in materials science and condensed matter physics because grain boundaries drastically affect the physical properties of polycrystalline materials. Thus the atom arrangement, termination plane, chemical composition, and electronic structure of grain boundaries, and in particular symmetric tilt grain boundaries, have been extensively investigated both experimentally and theoretically. In contrast, there are few studies of asymmetric tilt grain boundaries, despite being more prevalent, and therefore more significant to the material properties, than symmetric tilt grain boundaries.

In this presentation we introduce two symmetric and two asymmetric tilt [0001] Σ7 grain boundaries in Al_2O_3 through geometrical considerations. To find the stable grain boundary core structure, many configurations for each boundary were calculated using interatomic potentials. Interestingly, the grain boundary energies of the two asymmetric tilt grain boundaries are very similar to those of the symmetric tilt grain boundaries with the same Coincidence Site Lattice. We analyse the structures that emerge and compare the results with existing experimental data.

MM 33.3 Wed 12:15 TC 006

Deformation mechanisms of twinned Au-nanoparticles under compression: Experiments and Simulation — •Andreas Kelling[1], Cynthia A. Volkert[1], Wolfram Nöhring[2], and Erik Bitzek[2] — [1]Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen — [2]Lehrstuhl WWI: Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg, D-91058 Erlangen

The plastic deformation of nanoscale metallic specimens has recently attracted a lot of interest due to the reported changes of deformation mechanisms with reduced size. Here, we present compression experiments and atomistic simulations of gold nanoparticles to study dislocation processes and -storage in nanosized volumes. The particles are 80 and 250 nm in size and have faceted self-similar triangular shapes. They contain a twin boundary parallel to their upper and lower (111) surfaces. The particles are compressed along the [111] axis using a nanoindenter with a flat punch tip up to a strain of 50%. No dislocations were observed before deformation. Post-mortem TEM-analysis of both particle sizes reveals the storage of full dislocations. No difference in dislocation type is observed for the two different particle sizes. Molecular Dynamics simulations of Au particles with the same shapes were performed using different types of indenters and boundary conditions. The processes of dislocation nucleation, reactions, cross-slip and interactions with the twin boundary are studied in detail and analyzed in terms of the overall stress state. Comparison with the experimental microstructure allows us to draw conclusions about the dominant dislocation processes during the deformation of the particles.

MM 33.4 Wed 12:30 TC 006

Properties of fivefold twinned nanowires derived from microstructural constraints and anisotropic elasticity — •Florian Niekiel[1], Erdmann Spiecker[1], and Erik Bitzek[2] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute I: General Materials Properties, Department of Material Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg

Fivefold twinned metallic nanowires of fcc crystal structure have lately attracted a lot of attention because of their interesting properties and potential applications. Such nanowires consist of five segments, which are joined by {111}-twin boundaries, sharing a common crystal direction along the wire axis. The angular misfit of 7.35° resulting from joining the five wedge shaped segments necessitates the existence of a positive partial wedge disclination at the quintuple line present in the center of the nanowire. This peculiar microstructural constraint gives rise to significantly different properties of fivefold twinned nanowires in comparison to their single crystalline counterparts.

Here atomistic simulations and experimental diffraction measurements are combined to study the stress and strain state in fivefold twinned nanowires. Based on the findings a theoretical framework accounting for anisotropic elasticity is developed to quantitatively predict the mechanical properties of such nanowires as function of the used material. In this way the model helps not only to understand the properties of fivefold twinned structures but also to design their properties for future applications.

MM 33.5 Wed 12:45 TC 006

Mechanical and magnetic properties of Mn–Pt compounds and nanocomposites — •Tomáš Káňa[1] and Mojmír Šob[2,3,1] — [1]Institute of Physics of Materials, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [3]Faculty of Science, Masaryk University, Brno, Czech Republic

An analysis of mechanical and magnetic properties of Mn–Pt compounds and nanocomposites is provided using DFT calculations. Adding manganese to platinum matrix reduces the bulk modulus and enhances the Young moduli E_{100}, E_{111} as well as shear moduli (c_{11} - c_{12})/2 and c_{44}. With increasing Mn content, the theoretical tensile strength is also enhanced and the corresponding maximum deformation is reduced. On the whole, manganese addition makes the Mn–Pt compounds softer, but increases their resistance to shape deforma-

tion. Many of these compounds may be considered as natural linear nanocomposites. We studied the magnetic configurations of recently found $MnPt_7$ ordered structure and predict an antiferromagnetic state with spins altering along the [100] direction to be the ground state of this compound. We further studied Mn–Pt nanocomposites with the composition of $MnPt_{15}$. Here an antiferromagnetic structure with spins altering along the [100] direction is the ground state of $MnPt_{15}$ nanocomposite. The alternative ferromagnetic configurations of different $MnPt_{15}$ nanocomposites exhibit the screening of magnetic moments of Mn atoms by flipping the moments induced on Pt atoms into the opposite direction. This indicates that the Mn spins can be coupled through the Pt atoms.

MM 34: Topical Session Bulk Nanostrucured Materials VII - Mechanical Properties II

Time: Wednesday 11:45–13:00 Location: H 0107

MM 34.1 Wed 11:45 H 0107

The Effect of Severe Plastic Deformation on the Fatigue Behaviour of an Austenitic Stainless Steel — Oliver Renk, •Anton Hohenwarter, and Reinhard Pippan — Erich-Schmid-Institut, Leoben, Österreich

Ultra-fine grained and nanocrystalline materials produced by severe-plastic deformation represent a new class of materials as their properties can be varied over a wide range. Larger specimens now permit, the investigation of mechanical properties of these metals. However, only a few studies on structural materials, such as austenitic steels, exist. In this work the fatigue behaviour of a severely deformed 316L austenitic steel was investigated. By different processing parameters and a post heat treatment, four different ultra-fine grained and nanocrystalline structures were obtained, with grain sizes from 50 nm to 800 nm. The analysis of these different structures should allow a better understanding of the microstructural influence on the fatigue properties. Mechanical tests were conducted on the different severely deformed structures as well as on the coarse grained starting material to show the effect of severe plastic deformation. The main advantage of the ultra-fine grained austenitic structures compared with conventional heavily cold-rolled austenitic steels is, apart from their higher stress levels, their excellent cyclic stability. Fractographic Investigations showed completely different damage and fracture mechanisms of the ultra-fine grained and nano structures. Shear banding and strain localisation in these shear bands play a major role for the damage process during cyclic as well as monotonic loading.

MM 34.2 Wed 12:00 H 0107

Fatigue and crack propagation in SPD Cu with regard to microstructural stability — •Jelena Horky, Golta Khatibi, Brigitte Weiss, and Michael Zehetbauer — Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, 1090 Wien, Austria

For broad commercial applications of SPD nanomaterials not only enhancements in strength and ductility but also in fatigue and crack propagation are important. Therefore, this work aimed to investigate these properties in HPT (High Pressure Torsion)-processed Cu of two different purities. Besides high cycle fatigue (HCF), the main focus was laid on crack propagation. In case of cyclic loading, not only the thermal stability of HPT Cu but also its microstructural one is highly affected by the purity. Concerning high cycle fatigue, the reduced stability of a homogeneously nanostructured high purity Cu leads to grain coarsening and deteriorated fatigue strength. However, in case of very small load amplitudes and the presence of a crack, grain coarsening leads to retardation of crack growth, in contrast to a bimodally structured high purity Cu which shows a stable microstructure during crack propagation. Moreover, low purity HPT Cu which shows no grain coarsening during HCF, coarsens in the vicinity of a growing fatigue crack, indicating that crack propagation rates are determined by various, partly interdependent factors like purity, grain size, initial strength of the material and thermal stability of the microstructure.

The work has been supported by the Austrian Science Fund, under Project No. S10403.

MM 34.3 Wed 12:15 H 0107

Creep measurements in HPT-processed copper having ultrafine grain size — •Jörn Leuthold[1], Matthias Wegner[1], Anantha Padmanabhan[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Muenster, Germany — [2]School of Engineering Sciences & Technology, University of Hyderabad, India

In materials processed by severe plastic deformation, the presence of a high defect density in the form of dislocations, twins, high and low angle grain boundaries (GB) and their distribution affects the plastic deformation when a shear stress is applied. With a decrease in grain size into the sub-micrometer range, a dislocation-based deformation mechanism becomes increasingly unfavorable. Therefore GB diffusion and sliding account for the rate controlling deformation process even at low homologous temperatures, i.e. the creep resistance is significantly reduced. Regardless of the rate controlling physical mechanism, the "power law" is used to describe steady state, uniaxial deformation in the high stress, low homologous temperature regime. For this study copper samples were prepared by high pressure torsion and cut into a dog bone shape to perform isothermal tensile creep experiments. From load jump experiments, the stress exponent, activation energies for rate controlling flow and the strain rate values at different stresses and temperatures are obtained. Microstructural characterization in terms of nanoindentation, electron backscatter diffraction of as prepared and creep deformed specimens, changes in hardness, grain size distribution and texture are related to the observed activation energy.

MM 34.4 Wed 12:30 H 0107

Pressure dependence of plasticity in nanocrystalline Pd90Au10 — •Christian Braun, Manuel Grewer, 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 dominant shear-deformation. 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. The analysis of the pressure dependence of plastic flow relies on two prominent parameter, the pressure activation volume Δv_P and the Mohr-Coulomb coefficient μ. For nc Pd90Au10-samples with an average grain diameter of about 10 nm, we determined Δv_P to 1-2 b^3, where Δv_P is given as $\Delta v_P = \frac{\partial \sigma}{\partial P} \Delta v_\sigma$ and Δv_σ is the shear activation volume obtained from stress-strain-curves taken at different strain rates [2]. Applying the Mohr-Coulomb yield criterion, we deduced a friction coefficient μ in the order of 0.1-0.2 which is comparable to values obtained for a variety of bulk-metallic-glasses [3]. Analogies between the deformation behaviour of bulk-metallic-glasses and nanocrystalline materials in the limit of small grain sizes will be discussed.

[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), [3] Z.F. Zhang, J. Eckert, L. Schultz, Acta Mater. 51, 1167(2003)

MM 34.5 Wed 12:45 H 0107

Fracture behavior of copper: Ultrafine-grained vs. coarse-grained microstructure — •Anton Hohenwater and Reinhard Pippan — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, A-8700 Leoben, Austria

The fracture behavior of ultrafine-grained copper produced by high pressure torsion was evaluated by means of elasto-plastic fracture mechanics. The fracture toughness was quantitatively measured by JIC as a global measure by recording the crack growth resistance curve. As a local fracture parameter the initiation toughness in terms of the crack opening displacement (CODi) was evaluated by using an automatic fracture surface analysis system. The results show a remarkably high global fracture toughness, JIC, but at the same time a low fracture initiation toughness, Ji. In this contribution reasons for the large difference between these two parameters will be discussed and a comparison of the fracture mechanical performance of ultrafine-grained with coarse-grained copper will be given.

MM 35: Topical Session Theory meets Experiment III - Bond-order Potentials and Finite Temperature

Time: Wednesday 15:00–16:15 Location: TC 006

Topical Talk MM 35.1 Wed 15:00 TC 006

Simplified models of the electronic structure for predicting crystal structure stability — •Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Atomistic simulations may contribute to the theory-aided development of new materials mainly in two ways. Firstly, quantitatively accurate simulations of compound energies and properties may be used to screen materials across compositions and structures. Secondly, qualitative trends in structural stability and other properties may be explained and understood in terms of the bond chemistry and bond formation between the constituents of the material.

In this talk I will give examples for the combination of the two approaches and how they may be of help to suggest new experiments or contribute insight into the behaviour of materials. I will mainly focus on the stability of topologically close-packed phases in superalloys and the magnetic contribution to phase stability in iron and steels.

MM 35.2 Wed 15:30 TC 006

SAPIENS, a DFT and experimental based thermophysical database for pure elements — •Mauro Palumbo[1], Suzana G. Fries[1], Thomas Hammerschmidt[1], Ralf Drautz[1], Fritz Körmann[2], Tilmann Hickel[2], and Jörg Neugebauer[2] — [1]ICAMS, RUB, Stiepeler Str. 129, D-44801 Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany

Steels and Ni-based superalloys are multicomponent and multiphase materials. A theoretical approach for predicting phase stability as a function of composition, temperature and pressure for these materials should use the same method for all the phases since changes in potentials, approximations, etc can introduce differences which are of the same order of magnitude of the differences in energy required to describe the stability of real alloys. We developed a consistent first-principles database for Helmholtz energies from which thermophysical properties such as volume, heat capacity, bulk modulus, thermal expansion, can be calculated. Our approach took into account the contribution of different excitations (phonons, electronic excitations, magnons) for the temperature dependence. The vibrational contribution was evaluated within the Quasi-Harmonic Approximation. The electronic contribution was evaluated using Fermi-Dirac statistics and DFT based electronic Density of State. Magnetism was calculated using Heisemberg hamiltonian and Quantum Montecarlo. The methodology was applied to Fe, Cr, Ni, Al pure elements. Results were compared with an extended set of experimental data.

MM 35.3 Wed 15:45 TC 006

Bond-order potentials for bcc transition metals — •Miroslav Cak, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Bond-order potentials (BOPs) are based on the tight-binding approximation for determining the energy of a system of many interacting atoms. We present newly developed parametrisations of analytic BOPs for the refractory metals Tungsten, Molybdenum, Niobium and Tantalum. These metals play an important role as strengtheners of nickel-based superalloys and in topologically close-packed (TCP) phase precipitates in steels. Theory parameters of the analytic BOPs were optimised for the equilibrium bcc structure and extensively tested for atomic environments far from equilibrium that have not been included in the fitting procedure. These tests include structural energy differences for different competing structures; tetragonal, trigonal, hexagonal and orthorhombic deformation paths; formation energies of point defects and phonon dispersion relations. Comparing our calculations to corresponding first-principles, tight-binding and experimental results shows a very good transferability of our analytic BOPs to atomic structures encountered in lattice defects. From phonon densities of states we calculated heat capacities C_V at room temperatures that are in good agreement with experimental values. The new analytic BOPs were also applied to the calculation of melting temperatures using molecular dynamics simulations. Our results are in reasonable agreement with experiment and confirm that our BOPs capture the refractory character of W, Mo, Nb and Ta.

MM 35.4 Wed 16:00 TC 006

Computing atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron — •Fritz Körmann[1], Alexey Dick[1], Blazej Grabowski[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany — [2]Lawrence Livermore National Laboratory (L-280), P.O. Box 808, Livermore, California 94550, USA

Atomic forces are fundamental for using modern ab initio techniques in materials science. In this talk we propose a new methodological approach that allows to obtain atomic forces at finite magnetic temperatures solely from ab initio calculations. To demonstrate the power of the new approach we address a long standing but hitherto not solvable problem of computing phonon spectra for paramagnetic materials. As benchmark system we consider the experimentally well studied bcc and fcc phase of iron. The proposed scheme is general and an extension to study, e.g., systems containing defects (point or extended) or to combine it with molecular dynamic simulations is straightforward.

MM 36: Topical Session Bulk Nanostrucured Materials VIII - Functional Properties I

Time: Wednesday 15:00–16:30 Location: H 0106

Topical Talk MM 36.1 Wed 15:00 H 0106

Functional Nanomaterials by SPD: Hydrogen Storage, Shape Memory Effect, and Thermoelectricity — •Michael Zehetbauer[1], Maciej Krystian[1], Gerhard Krexner[2], Thomas Waitz[1], Gerda Rogl[1,3], and Peter Rogl[3] — [1]Physics of Nanostructured Materials, Vienna University, Austria — [2]Physics of Functional Materials, Vienna University, Austria — [3]Institute of Physical Chemistry, Vienna University, Austria

From recent efforts to functionalise bulk nanostructured materials, those of hydrogen storage, shape memory effect , and thermoelectricity revealed the strongest progress so far. For SPD processed ZK60 Mg alloy, the hydrogen adsorption/desorption rates are similar or even higher than those from milled nanomaterials. Also, loading/unloading processes are reproducible by at least 1000 cycles markedly exceeding the stability of milled nanomaterials. Controlled SPD processing of Shape Memory Alloys (SMAs) allows to affect not only the SME range but also their superelasticity, revocery stress and cyclic stability, paired with superior ductility and enhanced UTS. SPD processing of ferromagnetic SMAs has a strong impact on the kinetics of the martensitic phase transformation as well. Recently, SPD-mediated nanocrystallization reached record values for the efficiency of thermoelectric materials ('figure of merit ZT'). For p- and n-type skutterudites, HPT yields a marked reduction in grain size and increase in dislocation density. This decreases the thermal conductivity by 40% compared to conventionally milled skutterudites, and increases ZT by at least a factor 2. Work supported by FWF Austrian Science Fund under project S 10403

MM 36.2 Wed 15:30 H 0106

Magnetic Properties of nano-crystalline SPD treated SmFe2 — •Martin Kriegisch[1,2], Roland Grössinger[2], Reiko Sato-Turtelli[2], Frank Kubel[3], Daria Setman[1], Clemens Mangler[1], Martin Peterlechner[1], and Michael Zehetbauer[1] — [1]Physics of Nanostructured Materials, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Inst. of Solid State Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10; A-1040 Vienna, Austria — [3]Inst. of Chemical Technologies and Analytics, Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, Austria

High magnetostrictive materials are of great industrial importance, because of their potential application as magneto-mechanical sensor and actuator. The rare-earth intermetallic system SmFe2 exhibits a very high magnetostriction at room temperature. By adding a certain amount of Sm2O3 in the beginning of the melting process, we inhibited grain growth and produced nano-crystalline SmFe2 samples. Moreover we found that the addition of Sm2O3 also leads to a de-coupling of the exchange interaction between the nano-crystalline grains. As a consequence we proved that it is possible to tune SmFe2 from soft to hard-magnetic. After fully characterizing the magnetic and magnetostrictive properties, we investigated the effect of repeated cold-rolling (RCR) on the already nano-crystalline material. The changes of the magnetization and magnetostriction are analyzed and discussed with taking into account the internal stress and the stress-induced anisotropy. This work was supported by the FWF under the NFN-project numbers S10403 and S10406.

MM 36.3 Wed 15:45 H 0106

Magnetooptic Kerr Effect on severely deformed hard and soft magnetic materials — •Peter Jerabek[1], Reinhard Pippan[2], and Heinz Krenn[1] — [1]Karl-Franzens-University Graz, Graz, Austria — [2]Erich Schmid Institute , Austrian Academy of Sciences, Leoben, Austria

Magnetooptic Kerr effect (MOKE) is sensitive to the vector orientation of magnetization and offers a local probe of the domain structure. The high pressure torsion (HPT) of polycrystalline materials causes severe plastic deformation (SPD) [1] with a grain size refinement and a change of the magnetic domain structure (mostly a magnetic hardening). Ring specimens of different strain status (up to $\epsilon = 10$) are cut from HPT-deformed disk samples of ferritic steel and silicon-iron (Fe-3% Si). The boundaries between ultrafine grains (<100 nm) impede the motion of magnetic domain walls (accompanied by Barkhausen jumps) and pins the magnetization to preferred (textured) directions. The magnetic hysteresis measured by conventional induction method is compared with the local probe of polar, longitudinal and transverse MOKE (scanning the HeNe-laser spot over different parts of the HPT-ring sample). An interesting aspect is how SPD influences the strain-induced magnetization of originally magnetic soft Fe-3% Si and magnetic hard alloyed steels on the route from the polycrystalline to the dense nanocrystalline structure.

Financial support by the FWF Austrian Science Fund is appreciated (No. S10407-N16).

[1] M. Zehetbauer et al., Adv. Eng. Mat. 12 (2010), 692.

MM 36.4 Wed 16:00 H 0106

Strength and conductivity of graded Cu-particle reinforced aluminium processed by accumulative roll bonding — •Mathis Ruppert, Christian Werner Schmidt, Heinz Werner Höppel, and Mathias Göken — Institute I: General Materials Properties, Department Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Among the different processes of severe plastic deformation, accumulative roll bonding (ARB) is most prominent for production of ultrafine-grained sheet materials and has been studied extensively regarding microstructural evolution and mechanical properties. Besides the conventional ARB-processing route it is also possible to produce tailored multicomponent materials. In this context, particle reinforcement is of special interest, because of the manifold varieties of particles and distributions to tailor ultrafine-grained materials.

Applying particles in a highly controlled manner by air gun spraying from aqueous suspensions is used in this work as a method to introduce copper particles (d~1 micron) into aluminium AA1050A during ARB. Moreover it is demonstrated that the spatial distribution of particles within the sheet is widely controllable. Therefore homogeneous as well as continuously graded distributions can be achieved in all three dimensions of the sheet material. By this freedom of design, mechanical properties as well as electrical conductivity can be tailored rather locally within one sheet.

MM 36.5 Wed 16:15 H 0106

Hysteresis measurements of HPT treated Fe-Al — •Roland Grössinger[1], Nasir Mehboob[1], Martin Kriegisch[1,2], Reiko Sato-Turtelli[1], Andrea Bachmaier[3], and Reinhard Pippan[3] — [1]Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10/E138; 1040 Vienna, Austria — [2]Physics of Nanostructured Materials, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [3]Erich Schmid Institute of Materials Science, ÖAW Jahnstrasse 12, 8700 Leoben, Austria

Low cost magnetostrictive materials that exhibit a large magnetostriction at low saturation field combined with a high mechanical strength and a good ductility are of great interest for applications in magneto-mechanical sensors and actuators. Substituting Fe by non-magnetic Al causes a strong increase in magnetostriction mainly due to metastable equilibrium conditions among the disordered A2 and an ordered B2 and/or DO3 structure. The magnetostrictive properties of these alloys were already studied intensively in the past. For industrial applications the frequency dependent hysteresis properties (coercivity, permeability, losses) are of great importance. For this purpose the frequency behavior of the hysteresis loop of materials with enhanced magnetostriction was studied in a frequency range between 0.5 Hz and 200 Hz. Using this method the effect of a plastic deformation at different temperatures using the High Pressure Torsion (HPT) technique was investigated. The results were analyzed applying a new eddy-current based model on the frequency dependence of the coercivity as well as losses.

MM 37: Topical Session Modern Atom Probe Tomography I - Fundamentals

Time: Wednesday 15:00–16:45 Location: H 0107

Topical Talk MM 37.1 Wed 15:00 H 0107

A modelling approach to understand and improve image formation in Atom Probe Tomography — •François Vurpillot, Maria Gruber, Gérald Da Costa, Alain Bostel, and Bernard Deconihout — Groupe de Physique des Matériaux, UMR CNRS 6634, Université de Rouen, BP 12 , 76801 Saint Etienne Du Rouvray, France

The understanding of image formation in Atom probe Tomography is the direct consequence of the processes of field evaporation, emission and projection of ionised atoms from the Muller field emitter (a sharply pointed needle).

Basic models of field evaporation are now more than 50 years old. The models are extremely simple and ion trajectories are known to be governed by simple electrostatic relationships. Nevertheless, because since 30 years the complexity of materials analysed with the instrument has gradually increased (from simple metals to heterogeneous materials), these simple ingredients could give rise to various image artefacts. The comprehension of these artefacts and aberrations requires the use of numerical model to improve the fidelity of image reconstruction. This paper will show how the modelling approach could be used to understand the image deformations observed experimentally in complex devices or alloys. The role of temperature will also be discussed.

MM 37.2 Wed 15:30 H 0107

Multiscale 3D Simulation Of Atom Probe Measurements — •Christian Oberdorfer and Guido Schmitz — Institut für Materialphysik, Münster, Germany

A crucial step in atom probe tomography (APT) is the computer aided post processing of the raw measurement data in order to obtain 3D elemental distribution maps. In the case of modern instruments with improved field of view and due to distinguished properties for field evaporation these maps suffer from artifacts.

The talk will address this observation by presenting recent results from computer simulations.

Main features of the presented simulation scheme are the possibility to prepare arbitrary sample structures without any constraints on distinct lattice types or lattice orientations. The representation of single atoms by Wigner-Seitz cells allows even amorphous arrangements, and, in addition, also structural defects may be incorporated.

At the same time the foundation on an adaptive mesh allows the solution of the Poisson equation covering the mesoscopic scale with suited accuracy. This way, simulated ion trajectories reflect the experimental conditions and resulting datasets become comparable to experimental ones.

Topical Talk MM 37.3 Wed 15:45 H 0107

interaction between a field emitter and an ultra-fast laser beam — •Angela Vella, Jonathan Houard, Nicolas Sevelin-Radiguet, François Vurpillot, and Bernard Deconihout — Groupe de Physique des Materiaux UMR 6634 CNRS, Universite de Rouen Avenue de l'Universite,B.P. 12 76801 Saint Etienne du Rouvray Cedex, France

In laser assisted atom probe, the surface atoms of a field emitter (nanometric tip) are ionized by the combined action of a standing electric field and an ultra fast laser to trig the emission. The tip-laser interaction causes linear and non linear optical effects but also induces a heating of the tip. The evaluation of the absorption and heating of the field emitter becomes a key factor to compare the contribution to the evaporation process of the thermal and optical effects. In this contribution, we will present experimental methods and FDTD simulations (numerical solving of Maxwell equations) to determine the absorption properties of a metallic field emitter and the resulting evaporation behaviour. The dependence of these properties on the laser beam parameters (wavelength, polarization, power) will be studied. To conclude, the differences in the optical and evaporation behaviour between metallic and semiconductor or oxide field emitter will be discussed.

MM 37.4 Wed 16:15 H 0107

Atom probe tomography of solid state ion-conductive membranes — •Gerd-Hendrik Greiwe, Frank Berkemeier, Zoltan Balogh, and Guido Schmitz — Institut für Materialphysik WWU Münster, Münster, Germany

We could demonstrate that thin film membranes of amorphous Li-borate reveal a better conductivity than quenched bulk glasses (1). We measured the Li content by atom probe tomography. Layers of Li-borate and Li-silicate glasses were deposited upon tungsten tips. Although complex, the mass spectra are well understood in terms of various molecular species allowing a quantitative analysis. New effects at the interfaces were observed, that can be explained with the dielectric and ion-conductive properties of the glasses. By applying a base voltage to the specimen during the measurement, we create an electric field over the glass layer. Mobile Li ions redistribute to compensate the field. Therefore, we measure increased Li concentration at the surface and a depleted zone at the layer/substrate interface.

Using a model of field penetration and band bending by Tsong (2) we calculated the resulting electric field in the layers and its effect on the diffusion of the Li ions. This model predicts a field penetration of a few angstroems, forming a space charge surface layer. The calculations show reasonable agreement with the measurements, thus confirming the model.

(1) F. Berkemeier, M.R. Abouzari, G. Schmitz, Ionics, 15 (2009) 241
(2) T.T. Tsong Surface Science 82 (1979) 28-42

MM 37.5 Wed 16:30 H 0107

Investigation of optical properties of Silicon under high electric field by atom probe tomography — •Laurent Arnoldi[1], Angela Vella[1], Nicolas Sevelin-Radiguet[1], Francois Vurpillot[1], Tatiana Itina[2], Elena Silaeva[2], Nikita Shcheblanov[2], and Bernard Deconihout[1] — [1]Groupe de Physique des Matériaux, France — [2]Laboratoire Hubert Curien, France

In laser assisted atom probe, surface atoms are emitted from a tip in the form of ions by the combined action of an electrostatic standing field and a laser pulse that triggers the emission. The absorption of the light by the tip apex generates a pulse heat. Models have been proposed to explain the laser tip interaction and to evaluate the temperature rise and it spatial distribution on the specimen. In this contribution we will focus on the interaction between a silicon tip and an ultra-short laser pulse. New experimental methods to determine optical properties of the field emitter in real analysis conditions (very high electric field, cryogenic temperature) will be presented. Numerical solving of Maxwell equations allow predicting the changes of the tip's absorption when the illumination conditions are modified. These simulations incorporate the refractive index of the tip surface as derived from the calculation of the band bending effect on the surface that increases the density of free careers in the presence of the field. By comparing these simulations and experimental results, we will show that the absorption of a subwavelength tip is strongly dependent on the standing electric field applied to the sample.

MM 38: Liquid and Amorphous Metals

Time: Wednesday 15:00–17:00 Location: H 1029

MM 38.1 Wed 15:00 H 1029

Probing Shear-Band Initiation in Metallic Glasses — •David Klaumünzer, Robert Maass, Peter Thurnheer, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, ETH Zurich, Wolfgang-Pauli-Strasse 10, 8093 Zurich, Switzerland

At low homologous temperatures, metallic glasses are known to deform inhomogeneously by the formation of nanometer-sized shear bands. Typically, the operation of these bands is intermittent as reflected in serrated flow curves. This can be best understood in the context of stick-slip in which extended periods of arrest are followed by rapid slip events. The strong localisation of flow in space coupled with the fast operation of shear bands poses severe experimental challenges. We have approached this problem by using in-situ acoustic emission monitoring during compression testing of a Zr-based metallic glass. With this method, the mechanism of shear-band initiation prior to each slip event can be resolved. By drawing an analogy to the intermittent flow behaviour of granular media, we attribute the acoustic emission signal to a local volume expansion within a shear band. A quantitative analysis reveals volume changes for shear band initiation of a few percent only, in agreement with the excess free volume typical of the supercooled liquid regime.

[1] D. Klaumünzer et al., Physical Review Letters 107, 185502 (2011).

MM 38.2 Wed 15:15 H 1029

Size-dependent embrittlement in Zr-based bulk metallic glasses and its correlation to shear band velocities — •Peter Thurnheer, David Klaumünzer, Robert Maass, and Jörg Friedrich Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, 8093 Zürich, Switzerland

Despite extensive research during the last decades, plastic flow in metallic glasses remains a topic of intense debate. Since all metallic glasses are brittle in tension ($\epsilon_p < 0.5\%$), experimental focus lies on compression testing, where for some alloys, such as $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ (Vit105), several percent apparent plasticity can be observed. However, the amount of total plastic strain generated is found to depend highly on sample geometry, temperature and stiffness of both testing equipment and sample. Based on recent research that showed that one serration in the serrated flow regime of the stress-strain curve can be linked to the initiation, propagation and arrest of a single shear band, this work investigates the embrittlement of metallic glasses due to increasing specimen size, by analyzing the dynamics of single serrations with high temporal resolution. Samples with diameters ranging from 2 to 5 mm were tested. Similar to the case of metallic glass embrittlement as a function of increasing temperature, it was found that the total plastic strain to failure decreases with increasing sample diameter and that this decrease correlates with an increase of shear-band velocity during individual serrations.

MM 38.3 Wed 15:30 H 1029

Strain localization in amorphous Cu-Zr nanowires: Molecular dynamics simulations on the influence of size, surface relaxation state and temperature — •Yvonne Ritter and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstr. 32, 64287

Plastic deformation in bulk metallic glasses occurs at room temperature highly localized in narrow shear bands. Recent experiments, however, suggest a transition in deformation mode, from shear banding to a more homogeneous plastic deformation, if sample dimensions reach the nanometer regime. Despite the growing number of reports on size-dependent plasticity, doubts about the intrinsic nature of this size effect persist. When it comes to mechanical testing of nanoscale specimen, experimental artifacts can change the operating deformation mechanism.

In this study, cylindrical amorphous nanowires with diameters of 5-20 nm are studied by molecular dynamics simulations under tensile load. Two different amorphous alloys, a $Cu_{64}Zr_{36}$ and a $Cu_{36}Zr_{64}$ glass, are compared. By varying the surface relaxation state, temperature and sample diameter we find from the analysis of a statistically relevant number of samples no evidence for an intrinsic size-dependent transition in deformation mode. In both alloys, the occurrence of shear bands, neck formation or homogeneous flow is solely determined by the nucleation and coalescence of shear transformation zones exhibiting a size-independent activation free energy.

MM 38.4 Wed 15:45 H 1029

A model for superplastic deformation of metallic glasses — •Jonas Bünz[1], Gerhard Wilde[1], and K. Anantha Padmanabhan[2] — [1]Institut für Materialphysik, WWU Münster — [2]University of Hyderabad

The deformation behaviour of bulk metallic glasses is different from that of crystalline materials in that no restriction is placed on it that the displacement vector should be relared to the lattice parameter. Applied stresses get localized, lead to shear band formation and cause catastrophic failure after little or no plastic strain. In the supercooled liquid region, however, bulk metallic glasses can experience large strains; even superplasticity. We present a model for superplastic deformation of bulk metallic glasses, subjected to deformation in the supercooled liquid region. The model is based on the formation of shear transformation zones on a microscopic scale and the consequential development of mesoscopic glide planes of several nm. The model has been validated using experimental stress / strain rate data petaining to eight different glassy systems and is able to estimate the experimental strain rates within a factor of two. Based on this analysis the activation energy for rate controlling deformation and the threshold stress needed for the onset of interfacial sliding can be determined. Comparison with results obtained through other measurements reveals that the deductions based on the model are physically very meaningful.

MM 38.5 Wed 16:00 H 1029

Investigation of solidification dynamics of undercooled melts of Cu-Zr alloys — •Raphael Kobold[1], Dieter Herlach[1,2], and Ulrich Köhler[2] — [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

In contrast to experiments with most undercooled binary alloys the velocity of dendritic growth of a $Cu_{50}Zr_{50}$ alloy does not increase monotonically with undercooling but passes through a maximum and then decreases. To study this behaviour we investigate Cu-Zr alloys with Zirconium concentrations ranging from 44 to 54 at.% including eutectic and intermetallic phases. We use electrostatic levitation technique to melt and undercool samples with a diameter of 2-3mm under ultra-high-vacuum. Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures since heterogeneous nucleation on container walls is completely avoided. During crystallisation of the undercooled melt the heat of crystallisation is released. The rapid increase of the temperature at the solid-liquid interface makes the solidification front visible. The velocities of the solidification front are measured by using a high-speed camera with a maximum frame rate of 50 000 pictures per second. Furthermore, experiments for phase selection during rapid solidification of the undercooled Cu-Zr melts were performed at DESY Hamburg.

MM 38.6 Wed 16:15 H 1029

A study of phase separation in Zr-Gd-Co-Al metallic glasses — •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

The Zr-Co-Al and Gd-Co-Al ternary alloys are well known bulk metallic glass-former that could be cast into cylindrical rods with diameters up to 18 mm and 5 mm, respectively [1-2]. Since the binary Zr-Gd system has a miscibility gap in the solid state, i.e. Zr and Gd tend to separate from each other, the quaternary Zr-Gd-Co-Al system is a promising candidate to form phase separated glass-glass composites. In this work, Zr56-xGdxCo28Al16 (x = 2 - 20 at.%) melt-spun ribbons are characterized. The structure are further studied by In-situ small-angle and wide-angle X-ray scattering (SAXS/WAXS) at elevated temperature. Heat treated ribbons for x = 5 and 10 are additionally investigated by atom probe tomography. For ribbons with relatively low Gd content (x = 10 at. %), no indication for phase separation is found by general analysis such as SEM, XRD and DSC. In-situ SAXS/WAXS at elevated temperature gives evidence for formation of heterogeneity prior to crystallization. Atom probe tomography measurement also illustrates that the ribbons x = 5 and 10 undergo phase separation resulting in Gd-rich nano-scale precipitates prior to crystallization.

This study is supported by the Deutsche Forschungsgemeinschaft (Ma1531/10).

[1] T. Wada et al., J. Mater. Res, 24(2009)8
[2] D. Chen et al., Mater. Sci. Eng. A, 457(2007)226

MM 38.7 Wed 16:30 H 1029

Fraction of un-displaced atoms, structure conserving correlations, and temporal decay of structure fluctuations in simulated Ni0.5Zr0.5 melt — •Helmar Teichler — Inst. f. Materialphysik, Univ. Göttingen, Göttingen, Germany

The highly elaborated mode coupling theory provides a powerful tool to describe the temporal decay of fluctuations in melts. Notwithstanding this, there remains the question for the atomistic process behind the decay. To approach this problem, we analyzed simulation data of a Ni0.5Zr0.5 model close to its glass temperature at the accessible cooling rates. Recurring to our recent approach (H. Teichler, PRL, 107,067801 (2011)) we used as main tool the time evolution of the fraction of undisplaced particles (FUDP). The analysis shows that the alpha decay reflects the ultimate decrease of the FUDP. It irrefutably proves that the structural decay is due to temporal accumulation of incoherent short-ranged displacement events, where the stretched exponential behavior reflects structure conserving correlation in the accumulation process. In the contribution we present, in particular, a concise iteration procedure that describes the fluctuation decay over about eight decades from atomic vibrations to the beta and the alpha region.

MM 38.8 Wed 16:45 H 1029

Ultrafast Heating of Metallic Glasses using a Multistep Rapid Capacitor Discharge — •Stefan Küchemann[1], Jonas Rübsam[1], Carsten Mahn[1], Marios D. Demetriou[2], William L. Johnson[2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]Keck Engineering Laboratories, California Institute of Technology, Pasadena, California 91125, USA

Generally the study of the specific heat of metallic glasses is limited to temperatures below and close to T_G. The incipient crystallization process above the glass transition temperature prohibits the study of this quantity in the supercooled liquid region.

In this contribution specific heat measurements using a novel Multistep Rapid Capacitor Discharge (MRCD) technique are presented. With MRCD melt-spun Pd-, Ni- and Fe-based samples were heated up homogeneously with typical heating rates in the order of 10^6 K/s. The very high heating rates raise the stability of the undercooled melt and thus enlarge the temperature difference $\Delta T = T_X - T_G$ up to 400 K or even suppress crystallization completely.

After a first capacitor discharge the sample reaches the supercooled liquid region while under nearly adiabatic conditions additional discharges allow specific heat measurements in the undercooled liquid.

Financial support by DFG is gratefully acknowledged.

MM 39: Topical Session Theory meets Experiment IV - Batteries, Thermoelectrics and Thermal Barrier Coatings

Time: Wednesday 16:15–17:45 Location: TC 006

Topical Talk MM 39.1 Wed 16:15 TC 006

Electrode interfaces in organic electronics — •Karsten Albe, Peter Agoston, Andre Wachau, Mareike Hohmann, and Andreas Klein — TU Darmstadt, Inst. für Materialwissenschaft, Petersenstr. 32, D-64287 Darmstadt

Sn-doped In_2O_3 (ITO) is a transparent conducting oxide with a high transparency in the visible range of the optical spectrum and high electrical conductivity, which is widely used as transparent electrode material for organic light emitting diodes and organic photovoltaics. Due to the orientation dependent ionization potential, a polycrystalline ITO film will exhibit a laterally varying work function, which results in an inhomogeneous charge injection into organic semiconductors when used as electrode material. Thus, a detailed understanding of the surface structure and thermodynamics is a prerequisite for optimizing the transparent electrode. In this contribution the thermodynamic stability of several experimentally observed low-index surfaces of bcc indium oxide (In2O3) are investigated by means of density functional theory calculations. The influence of hydrogen, water, n-type dopants (Sn), as well as the in-plane lattice strain are studied and compared to results of STM-studies on single crystalline samples. The computed data are also contrasted with results from photoelectron spectrocscopy on magetron-sputtered layers and explain, why the orientation dependence of the work function will become even more pronounced when oxygen plasma treatments are performed.

MM 39.2 Wed 16:45 TC 006

Current theoretical investigations of Li_xSi as electrode materials in Li-Ion-Batteries — •Thomas Gruber and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

Li_x Si may be a promising anode material for lithium ion batteries. We will discuss the crystal structures of the known stable phases and will identify similar structural elements. In particular using the electron localization function (ELF) we will investigate the bonding in these structures. The main goal of our investigation is to support an understanding of the charging and discharging processes, which are directly related to the Li^+ transport.

For any application of Li_x Si as anode material a proper understanding of the thermodynamical behavior of the material is required. The calculation of the complete phonon dispersion as function of pressures allows for the construction of the Gibbs free energy, which then gives access to specific heat or other thermodynamical data. The Gibbs free energy and derived thermodynamical quantities can be used for thermodynamical modeling of Li-ion batteries or as input for phase field simulations.

MM 39.3 Wed 17:00 TC 006

First Principles Study of Thermoelectric Boron-Carbide Compounds — •Karsten Rasim, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin

A significant fraction of the world energy consumption goes into "waste heat". For recovering some of it one needs to develop significantly more efficient thermoelectric (TE) materials then what is known to date. Boron-carbide based compounds have recently been proposed as promising candidates for high temperature applications, in particular due to the fact that their TE properties can be remarkably altered by adding a large variety of rare earth or transition metals [1]. In this work, we employ *density functional theory* (DFT) to assess the electronic and atomistic structure of such modified boron-carbide compounds. Thereby, we are able to identify the elemental mechanisms that determine the properties of these materials, e.g., the sign of the majority charge carrier [1]. We further discuss how the systematic underestimation of the band gap with approximate *exchange-correlation* (XC) functionals [2] affects our results by comparing experimental data and calculations performed at various levels of theory, i.e., with LDA, GGA, and hybrid XC functionals. In particular, we comment on the implications of these findings with respect to the computational assessment of TE properties [3].

[1] T. Mori and T. Nishimura, *J. Sol. State Chem.* **179**, 2908 (2006).
[2] P. Rinke *et al.*, *New J. Phys.* **7**, 126 (2005).
[3] P. Boulet *et al.*, *Comp. Mat. Sci.* **50**, 847 (2011).

MM 39.4 Wed 17:15 TC 006

Computational study of structures of yttria-stabilised zirconia/strontium titanate multilayers — •Wei Li Cheah and Mike Finnis — Imperial College London, UK

Growing interest in the field of functional oxide multilayered nanoheterostructures may be attributed to their unusual interfacial properties that are not yet fully understood. For instance, the nature of the unexpectedly high conductivity reported in a trilayer of 1-nm thick epitaxial yttria-stabilised zirconia (YSZ) film sandwiched between strontium titanate (STO) layers [1] still remains controversial. In an effort to investigate the source of conductivity in this system, we first establish an unexpected YSZ lattice within such heterosystem using a combination of techniques - a genetic algorithm in which the interatomic forces are described by classical pair potentials, and a pseudopotential-based DFT method as implemented in the plane-wave code CASTEP. We find this structure to be more stable than an anatase zirconia epitaxial lattice on STO which has been previously found as the most stable structure if yttrium dopants were not incorporated within the zirconia layer. Analysis of charge density of this new structure reveals not localised vacancies, but several small pockets of low charge densities for each expected vacancy. We examine the mobility of oxide ions in the heterosystem using classical molecular dynamics simulation and attempt to relate the results to experimental conductivity values.

[1] J. Garcia-Barriocanal et al., Science, vol. 321, no. 5889, pp. 676-680, 2008.

MM 39.5 Wed 17:30 TC 006

Phase Stability in Yttria-stabilized Zirconia from First Principles — •Christian Carbogno[1,2], Carlos G. Levi[1], Matthias Scheffler[1,2], and Chris G. Van de Walle[1] — [1]Materials Department, University of California, Santa Barbara, CA 93106-5050, USA — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany

Zirconia based ceramics are of pivotal importance for a variety of industrial technologies, e.g., for *thermal barrier coatings* in gas and airplane turbines [1]. Naturally, the stability of such coatings at elevated temperatures plays a critical role in these applications. It is well known that an aliovalent doping of tetragonal ZrO_2 with Yttria, which induces oxygen vacancies due to charge conservation, increases its thermodynamic stability [1, 2]. However, the atomistic mechanisms that determine the phase stability of such *Yttria-stabilized Zirconia* (YSZ) coatings are not yet fully understood [2]. In this work, we use *density functional theory* calculations to assess the electronic structure of the different YSZ polymorphs at various levels of doping. With the help of population analysis schemes, we are able to unravel the intrinsic mechanisms that govern the interaction in YSZ and that can so explain the relative stabilities of the various polymorphs. We critically compare our results to experimental measurements and discuss the implications of our findings with respect to other oxides.

[1] A. G. Evans, D. R. Clarke, and C.G. Levi, *J. Eur. Ceram. Soc.* **28**, 1405 (2008).
[2] J. A. Krogstadt et al., *J. Am. Ceram. Soc.* **94**, S168 (2011).

MM 40: Topical Session Bulk Nanostrucured Materials IX - Functional Properties II

Time: Wednesday 16:30–17:45 Location: H 0106

MM 40.1 Wed 16:30 H 0106

Crack formation during dealloying of Au25Cu75 — •Yi Zhong[1], Haijun Jin[2], and Jörg Weissmüller[1,3] — [1]Helmholtz Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, Germany — [2]Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China — [3]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und Technologie, Germany

Alloy corrosion has recently evolved into a method for making nanoporous metal materials. The dealloying process, however, often produces cracks which develop during the concurrent shrinkage. Here, we explore a new strategy to reduce the volume shrinkage while retaining small structure size. The idea is to start with a master alloy (e.g., Au25Cu75) which has smaller lattice spacing than that of the nanoporous product (Au), expecting that the lattice expansion during dealloying will compensate the shrinkage. Most interestingly, unlike the monotonically increase of shrinkage with increasing dealloying potential as observed in Au25Ag75, the copper-based system has a maximum volume shrinkage and the highest density of cracks for dealloying at intermediate potentials. Besides, other pretreatment procedures such as High Pressure Torsion (HPT) or cancellation of recovery heating could also effectively eliminate the cracks which usually propagate along grain boundaries. Therefore, at high dealloying potentials one obtains samples with almost no crack and concurrently smaller structure size, offering a unique opportunity to develop new nanoporous materials with combined high functionality.

MM 40.2 Wed 16:45 H 0106

About strain homogeneity at HPT in ufg and nc Pd — •Lilia Kurmanaeva[1], Yulia Ivanisenko[1], Aaron Weis[1], Christian Kübel[1], Delphine Chassaing[1], and Hans-Jörg Fecht[1,2] — [1]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology, Germany — [2]Institute of Micro and Nanomaterials, University of Ulm, Ulm, Germany

It is known that ufg and nc are prone to the localization of deformation, which leads to the lack of ductility in tension. However, strain inhomogeneity also takes place during torsion straining. Since high pressure torsion is very important method to produce nanostructured samples, here we studied deformation homogeneity at HPT of ultrafine-grained and nanocrystalline Pd and Pd alloys in radial direction. Disk samples were cut at a middle of radius. On the electrolytically polished cut surface a fine grid was produced by FIB. Then samples were HPT strained. We observed an obvious strain localisation on the deformed grid in ufg samples. For a further investigation plane-view TEM samples were cut from the area of the grid. The obtained results of TEM microstructure of Pd and Pd alloys are discussed.

MM 40.3 Wed 17:00 H 0106

Diffusion in α-titanium after severe plastic deformation — •Jochen Fiebig[1], Sergiy Divinski[1], Yuri Estrin[2], Ruslan Valiev[3], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälische Wilhelms University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institute of Physics of Advance Materials, Ufa State Aviation University, 12 K. Marx Street 450000 Ufa, Russian Federation — [3]Department of Materials Engineering, Monash University, Clayton, Victoria 3800, Australia

In the present study we focus on the diffusion and mechanical properties of severely deformed α-titanium produced by equal channel angular pressing (ECAP), including continuous ECAP, and high-pressure torsion. The radiotracer method in combination with parallel sectioning was used to study the self-diffusion (^{44}Ti radioisotope) and solute diffusion of silver (^{110m}Ag radioisotope). The diffusion data were analyzed with regard to the different production methods of ultrafine grained Ti and their potential for generating a special, "non-equilibrium" state of general high-angle grain boundaries. Such interfaces should exhibit a higher diffusivity than general high-angle grain boundaries in coarse grained Ti. The microhardness and its variation with temperature were measured to analyze the stability of the microstructure of the material. The microstructure was studied by TEM and SEM analyses, including EBSD measurements.

MM 40.4 Wed 17:15 H 0106

Irradiation tolerance of bulk nanocrystalline alloys — •Askar Kilmametov[1], Kay Potzger[2], Christoph Gammer[3], Mohammad Ghafari[1,4], Ruslan Valiev[5], and Horst Hahn[1,4] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]University of Vienna, Physics of nanostructured materials, Vienna, Austria — [4]Institute for Materials Science, Joint Research Laboratory Nanomaterials, Darmstadt, Germany — [5]Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Ufa, Russia

Radiation effects in nanostructured materials have attracted increasing interest in materials science. Bulk ordered nanocrystalline TiNi and FeAl alloys were processed using high pressure torsion. Fully-dense nanocrystalline and coarse-grained counterparts possessing a long-range ordering studied by X-ray diffraction and Mössbauer spectroscopy to examine irradiation effects on the stability or degradation of crystal superlattice. Comparative analysis of long-range disordering and amorphisation kinetics revealed essentially enhanced irradiation resistance of nanocrystalline intermetallic alloys. It was shown that at the equal damage dose nanocrystalline samples are able to retain a long-range ordering while the coarse-grained counterparts were substantially disordered or amorphised. The present experimental studies verify that fully-dense ordered intermetallic alloys are promising candidate materials for radiation environments.

MM 40.5 Wed 17:30 H 0106

Short-Circuit Diffusion in Ultrafine-Grained Copper Processed 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, WWU Münster, Wilhelm-Klemm-Straße 10, D-48149 Münster, Germany — [2]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria

Short-circuit diffusion paths in ultrafine-grained copper processed by High Pressure Torsion are investigated by the radiotracer method. *Ultra fast* diffusion rates in addition to *conventional* rates of grain boundary (GB) diffusion are observed. The *ultra fast* diffusion is related to a so-called *non-equilibrium* state of GBs. According to existing models of grain refinement by severe plastic deformation, the abundance of lattice dislocations created during the severe straining serves to modify the structure of high angle GBs towards a non-equilibrium state with an enhanced excess free energy density. The kinetic and structural properties of these *non-equilibrium* GBs are thoroughly investigated and compared with previous results obtained on Cu and Cu alloys deformed by Equal Channel Angular Pressing. Furthermore, a network of percolating porosity is observed. This unexpected feature resembles previously discovered porosity in ECAP processed Cu. A strong dependence of the volume fraction of the porosity on the processing parameters is elucidated. The anisotropy of the percolating porosity is examined with respect to the shear direction.

MM 41: Topical Session Modern Atom Probe Tomography II - Functional Materials

Time: Wednesday 16:45–17:45 Location: H 0107

MM 41.1 Wed 16:45 H 0107

Impurity distributions in Cu(In,Ga)Se_2 thin-film solar cells studied by Atom Probe Tomography — •Ralf Schlesiger[1], Roland Würz[2], Jens Bastek[1], Katharina Hiepko[1], Nicolaas A. Stolwijk[1], and Guido Schmitz[1] — [1]Institute of Material Physics, Westf. Wilhelms-Universität Münster, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Germany

To improve and understand the benchmarks of polycrystalline thin-film solar cells based on the compound semiconductor Cu(In,Ga)Se_2, detailed knowledge of the atomic-scale distribution of minority impurities is desirable and can only be obtained by atom probe tomography. During the growth process of the absorber at about 600°C, diffusion of impurity atoms from the substrate through the Mo back contact into the absorber layer is observed, affecting the efficiency of the absorber layer. In this work atom probe measurements were carried out to analyse the distribution of Na, Fe and Cd impurities within the Cu(In,Ga)Se_2 absorber layer. Na was exclusively introduced during crystal growth, whereas Cd and Fe were diffused at temperatures below 550°C from the front side of as-grown CIGS layers. It is clearly resolved that Na is mostly localized in the grain boundaries. While Fe is homogeneously distributed in the grain volume, with no enrichment at the grain boundaries, Cd shows a slight segregation to the grain boundaries. Concerning the Cu(In,Ga)Se_2 constituents at the grain boundaries, a depletion was found for Cu, with a simultaneous enrichment of In and Se.

MM 41.2 Wed 17:00 H 0107

Exploring the internal interfaces at the atomic-scale in Cu(In,Ga)Se2 thin-films solar cells — •Oana Cojocaru-Mirédin[1], Pyuck-Pa Choi[1], Roland Wuerz[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany

Cu(In,Ga)Se2 solar cells possess a high efficiency, despite the polycrystalline structure of the absorber layer. This is mainly due not only to the impurities diffusion from the soda-lime glass substrate inside the absorber layer, but also to the CdS/Cu(In,Ga)Se2 p-n junction. However, the recombination mechanism between the defects and the impurities at the internal interfaces remains far to be understood. This is due to a lack of information on local chemical changes across the internal interfaces at the nanoscale. In this work, the internal interfaces, CdS/Cu(In,Ga)Se2 interface and Cu(In,Ga)Se2 grain boundaries, were explored at atomic-scale by means of atom probe tomography. A Cu-depleted and Cd-doped region (~ 2 nm in width) was detected at the Cu(In,Ga)Se2 surface. It was also shown that Cd diffused through the Cu(In,Ga)Se2 grain boundaries during the deposition of CdS layer. The diffusion of Cd inside the Cu(In,Ga)Se2 grain, but also in the grain boundaries prove the existence of a buried p-n homojunction within the Cu(In,Ga)Se2 absorber layer. Regarding the Na (K) and O impurities, they were found to decorate not only the CdS/Cu(In,Ga)Se2 interface, but also the Cu(In,Ga)Se2 grain boundaries. The present results were compared with the existing electronic GB models.

MM 41.3 Wed 17:15 H 0107

Nanoanalysis of CoFeB electrodes in pseudo spin valve magnetic tunnel junction — •Houari Bouchikhaoui, Patrick Stender, Mohammed Reda Chellali, and Guido Schmitz — Institut für Materialphysik der WWU, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

A magnetic tunnel junction (MTJ), which consists of a thin insulator layer sandwiched between two ferromagnetic electrode layers, exhibit tunnel magnetic resistance TMR due to spin-dependent electron tunnelling. The theoretical prediction of over 1000% TMR by the preferential tunnelling of $\Delta 1$ Bloch states in Fe/MgO/Fe magnetic tunnel junction led to the experimental demonstration of giant TMR about 150% at room temperature. The pseudo spin valve PSV MTJs $Ta/Co_{20}Fe_{60}B_{20}/MgO/Co_{20}Fe_{60}B_{20}/Ta$ has great interest due to high magnetoresistance TMR value at room temperature after annealing at elevated temperatures. In this work, we analysed the nanostructure and chemical distribution of constituent elements in $Ta/Co_{20}Fe_{60}B_{20}/MgO/Co_{20}Fe_{60}B_{20}/Ta$ PSV MTJs annealed between room temperature and 600C° by atom probe tomography (TAP). The segregation of Boron to the interfaces will be presented in dependence on temperature.

MM 41.4 Wed 17:30 H 0107

Atom Probe Tomography of ONO stacks for in-production flash memory — •Sebastian Koelling[1], Ahmed Shariq[1], and Sonja Richter[2] — [1]Fraunhofer Center Nanoelectronic Technologies, Königsbrücker Straße 180, 01099 Dresden, Germany — [2]X-FAB Dresden GmbH & Co. KG, Grenzstrasse 28, 01109 Dresden, Germany

The introduction of laser assisted Atom Probes with a wide angle detector systems made Atom Probe Tomography a highly interesting technique for routine analysis of semiconductor devices. While laser assisted Atom Probe analysis of bulk semiconductors like silicon or germanium is nowadays routinely possible, the analysis of insulating layers is still challenging even with the most recent generation of tools. As insulating oxide and nitride layers are an integral part of the gate of every transistor, we are working on overcoming this limitation. Here we will report on our progress in analyzing gate stacks for state-of-the art transistor structures. We will focus on (silicon-) oxynitride/oxide stacks used in present-day flash memory. These stacks are 10-20 nm thick and are particularly challenging to analyze due to their comparatively large thickness and the need for mapping the nitrogen content inside the layers. We will present ways to improve the yield when measuring these stacks and an approach to quantify the nitrogen in-spite of the mass overlap with silicon.

MM 42: HV Spiecker

Time: Wednesday 18:00–18:30 Location: H 0107

Invited Talk MM 42.1 Wed 18:00 H 0107

In-situ Transmission Electron Microscopy of Phase Transformations in Materials — •Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen

Over the past decades transmission electron microscopy (TEM) has established itself as a powerful tool for investigation of phase transformations in materials. The unique capability of combining electron diffraction with chemical analysis and structural imaging at high resolution makes TEM particularly suited for studying local material transport and the role of defects and interfaces in phase transformations. In this presentation examples of in-situ TEM studies of phase transformations will be discussed including metal-induced crystallization (MIC) of elemental semiconductors in thin film stacks and structural transformations associated with the metal-to-insulator transition (MIT) in VO2. In MIC grain boundaries and built-up of stress turn out to play a key role in crystallization and related material transport. In the case of MIT the importance of defects and geometric contraints for the occurence of hysteresis will be discussed.

MM 43: HV Hickel

Time: Wednesday 18:30–19:00 Location: H 0107

Invited Talk MM 43.1 Wed 18:30 H 0107

Advancing ab initio methods to finite temperatures for applications in materials design — •Tilmann Hickel, Alexey Dick, Fritz Körmann, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The performance of materials such as steels, their strength and formability, are based on an impressive variety of competing mechanisms on the atomic/microscopic scale, ranging from point defects up to mechanical twinning or structural phase transformations. Whereas many of these mechanisms are currently described with empirical concepts and experimental data, it becomes more and more apparent that further improvement of materials needs to be based on fundamental theories. Recent progress in the field of ab initio methods now makes the exploration of chemical trends, the determination of parameters for phenomenological models and the identification of new routes for the optimization of material properties feasible. A major challenge in applying these methods to a true materials design is, however, the inclusion of temperature-driven effects on the desired properties. This talk will, therefore, address the large range of computational tools we have developed in order to improve the capability and accuracy of first-principles methods in determining free energies. These combine electronic, vibrational, and in particular magnetic excitations, but also structural defects in an integrated approach. Based on these simulation tools, we are able to successfully predict with a hitherto not achievable accuracy mechanical and thermodynamic properties of metals, such as high-strength steels and magnetic shape-memory alloys.

MM 44: HV Hugenschmidt

Time: Thursday 9:30–10:00 Location: H 0107

Invited Talk MM 44.1 Thu 9:30 H 0107

Positrons Probing Matter: Bulk and Thin Film Studies Using the Low-Energy Positron Beam at NEPOMUC — •Chrisotph Hugenschmidt — Technische Universität München

Experiments using positrons as microprobes allow the investigation not only of lattice defects but also of their chemical surrounding. Thin films as well as the bulk of samples can be studied using a low-energy mono-energetic positron beam. The defect sensitive Doppler broadening spectroscopy (DBS) of the annihilation line is well suited to perform spatially resolved defect maps. Moreover, due to the large background suppression the coincident mode (CDBS) enables the non-destructive examination of the elements involved in the annihilation process.

As examples, studies on plastically deformed samples of Al alloys and on irradiated materials will be presented. In addition, recent depth dependent experiments on defect annealing in thin Cu-layers and on temperature dependent alloying of thin CuAu-films will be presented. It is demonstrated how the formed phase can be determined by comparison with theoretically calculated annihilation spectra.

Within this presentation, an overview of the beam facility at the neutron induced positron source NEPOMUC and the positron instrumentation is given as well. Future developments and applications of the high-intensity positron beam will be discussed.

MM 45: Computational Materials Modelling VI - Thermal Conductivity and Transport

Time: Thursday 10:15–11:45 Location: TC 006

MM 45.1 Thu 10:15 TC 006

Thermal Conductivities at High Temperatures from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at *high temperatures* has remained elusive. Under such conditions, techniques that rely on the harmonic approximation become questionable, while non-equilibrium MD methods require huge temperature gradients that lead to undesired non-linear effects. The Green-Kubo method, which does not suffer from these shortcomings, involves the assessment of the thermal conductivity from the auto-correlation of the heat flux via equilibrium MD. This method has hitherto been disregarded in first-principles simulations since the computation of the heat flux requires the energy contributions from the individual atoms, a quantity that is not directly accessible in first-principles schemes. We show that the Green-Kubo approach can be reformulated in terms of the *energy density* [1], which is directly accessible in density functional theory calculations. This approach leads to a unique definition of the heat flux that does not rely on any partitioning scheme for the total energy. To demonstrate the capabilities of this technique, we investigate the thermal conductivity of ZrO_2, a material that is widely used in industrial high-temperature applications.

[1] N. Chetty and R. M. Martin, *Phys. Rev. B* **45**, 6074 (1992).

MM 45.2 Thu 10:30 TC 006

Thermal conductivity of minerals at the Earth's core-mantle boundary from equilibrium molecular dynamics — •Volker Haigis[1], Mathieu Salanne[2], and Sandro Jahn[1] — [1]GFZ German Research Centre for Geosciences, Telegrafenberg, 14473 Potsdam, Germany — [2]UPMC Université Paris 06 and CNRS, UMR 7195, PECSA, 75005 Paris, France

The thermal conductivity at the Earth's core-mantle boundary is an important geophysical parameter which governs the heat flux across the boundary and thus influences the dynamics of both core and mantle. However, conductivities at the relevant temperatures and pressures cannot be measured with present-day experimental techniques. Hence a computational approach is desirable. We report thermal conductivities of fcc MgO and $MgSiO_3$ in the perovskite and the post-perovskite structure at conditions representative of the Earth's lowermost mantle, obtained from equilibrium molcular dynamics. Using an advanced ionic interaction potential [1], the full conductivity tensor was calculated by means of the Green-Kubo method, and the conductivity of $MgSiO_3$post-perovskite was found to be significantly anisotropic. Assuming an iron-free mantle composition with $x_{MgSiO_3} = 0.66$ (in the post-perovskite structure) and $x_{MgO} = 0.34$, we predict the average thermal conductivity at the core-mantle boundary to be (24.3 ± 1.8) W/(mK). Based on experiments [2], we expect that a realistic amount of iron impurities reduces the conductivity to (12 ± 1) W/(mK).

[1] S. Jahn, P. A. Madden, Phys. Earth Planet. Int. **162**, 129 (2007)
[2] G. M. Manthilake *et al.*, PNAS **108**, 17901 (2011)

MM 45.3 Thu 10:45 TC 006

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

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

For computational studies of dynamic properties long simulation times and large samples are required. This makes first principle calculations of these structures, even with high performance computers, very unfeasible. Classical molecular dynamics, however, can meet the

requirements. 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 reproduces 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. With this potential and the Green-Kubo method, the thermal transport in different Ge-based clathrate systems has been investigated.

MM 45.4 Thu 11:00 TC 006

Ab initio characterization of thermoelectrical materials — •Matthieu Verstraete — Nanomat unit, Physics Department University of Liege, Belgium

Energy production, storage, and efficiency have become pressing issues in society, science, and materials in particular over the past few decades. Thermoelectrical materials are a classical technology which may come into its own thanks to advanced nanostructuring and controlled alloying. Understanding the microscopic mechanisms which can improve on efficiencies of bulk materials is crucial. We will present the ab initio DFT characterization of thermoelectrics with very different mechanisms, behaviors, and relevant temperature ranges, in particular Mg2Si and FeSb2. Specific unsolved issues in the theoretical treatment of thermoelectrics will be raised and discussed.

MM 45.5 Thu 11:15 TC 006

Transport properties of nanoconfined water — •Akinlolu Akande[1], Ivan Rungger[1,2], Clotilde Cucinotta[1], Konstantinos Gkionis[2], Udo Schwingenschlögl[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, TCD Dublin, IRELAND — [2]KAUST, Saudi Arabia

Understanding the electronic transport properties of nanoconfined systems under wetting conditions is essential for many applications, ranging from molecular nano-junctions to nano-electronics. Here we focus on the transport properties of water confined between a gold STM tip and a gold surface. We perform calculations for the molecular dynamics of the water and quantum transport simulations for a randomly selected set of time-snapshots. These are at the level of the non-equilibrium Green function method, as implemented in the SMEAGOL code. We calculate the dependence of the conductance in liquid water on the separation between the confining surfaces, and find good agreement with experimental findings.

Within the electron tunnelling regime we study the dependence of transport properties of the nanoconfined system on liquid water, also comparing it with the transport in vacuum. The dependence is explained further in terms of the complex band structure of water, which determines - together with the interface structure - the decay of the conductance with thickness. This study allows us to unravel the relationship between conductance and the microscopic structure of nanoconfined water and explores the possibility to detect the phase of a water sample by current measurements.

MM 45.6 Thu 11:30 TC 006

Quantum transport simulations in metallic carbon nanotubes with metal contacts — •Andreas Zienert[1], Jörg Schuster[2], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, Chemnitz University of Technology, 09126 Chemnitz, Germany — [2]Fraunhofer Research Institution for Electronic Nano Systems, 09126 Chemnitz, Germany

Carbon nanotubes (CNTs) are one dimensional conductors with promising applications in future microelectronic devices and sensors. Due to their high thermal and mechanical stability and their ability to carry high current densities, they are discussed as novel interconnect materials, partially replacing copper metallization in future microelectronic devices. However, the performance will strongly depend on the quality of contacts between CNTs and the environment [1].

The geometric structure of CNT-metal contacts is modeled using density functional theory. A simple approach for contact geometry optimization will be presented. Non-equilibrium Green's function methods in combination with DFT are used to study electronic transport through metal–CNT–metal devices. Results for different metals will be interpreted in terms of electronic properties of the bulk materials and the contact area.

[1] Zienert et al. Phys. Stat. Sol. B 247, 3002 (2010)

MM 46: Nanomaterials I

Time: Thursday 10:15–11:45 Location: H 1029

MM 46.1 Thu 10:15 H 1029

SiC formation in carbon nanotubes grown from permalloy catalyst particles — •Anja Kiessling[1], Darius Pohl[1], Christine Täschner[1], Rolf Erni[2], Mark Hermann Rümmeli[1], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Carbon nanotubes (CNT) were grown from $Ni_{80}Fe_{20}$ ("permalloy") catalyst particles on Si substrates using plasma-enhanced chemical vapour deposition (PE-CVD). The as-produced CNT were characterized by means of aberration-corrected high resolution transmission electron microscopy (using a FEI TITAN^3 80-300 microscope operated at 80kV). The as-grown CNT exhibit a clear contrast difference between the particle, the concentric graphene layers of the CNT and their cores. Electron Energy Loss (EEL) spectra reveal the core to be SiC from the occurrence of a Si-L absorption edge at around ΔE=100eV followed by a broad double-peak. Furthermore the CNT are found to be covered by a SiO_2 layer. The SiC core is expected to form during CNT growth as well as a Si film around the CNT due to the presence of Si in gas phase. This then oxidizes during exposure to ambient air. In summary, the CNT exhibit a complex core-shell structure consisting of a SiC core, a shell of concentric graphene layers and an amorphous SiO_2 overcoat.

MM 46.2 Thu 10:30 H 1029

Evolution of nanoporosity via dealloying in binary and ternary Pt alloys — •Henning Galinski[1], Thomas Ryll[1], Yang Lin[1], Ludwig J. Gauckler[1], and Max Döbeli[2] — [1]Nonmetallic Inorganic Materials, ETH Zurich, Zurich, Switzerland — [2]Ion Beam Physics, ETH Zurich, Zurich, Switzerland

The controlled tailoring of nano-porosity in metallic thin films of several 100 nm thickness using dealloying has gained renewed attention in recent years, as such nanoporous thin films are candidates for applications in sensors, micro-fuel cells and super-capacitors. In this contribution the physical mechanism of nanoporosity formation during the dealloying process of binary PtAl- and ternary PtYAl-alloy thin films is examined using focused ion beam (FIB) nanotomography and Rutherford backscattering spectrometry (RBS). The dynamics of nanoporosity formation is found to obey a superposition of a reaction-diffusion equation describing a linearly propagating diffusion front[1] and a secondary slower dissolution process away from the moving interface. An increased Al content as well as a partial substitution of Pt by Y results in a slower dealloying kinetics with a slower linearly propagating diffusion front. The resulting nanoporous Pt thin films perform exceptionally well as oxygen reduction electrodes in a micro-solid oxide fuel cell setup[2] in the temperature range from 473 to 1073 K.

[1] PRL 107, 225503 (2011), [2] PRB 84, 184111 (2011)

MM 46.3 Thu 10:45 H 1029

Metallic nanowire growth from solution using dielectrophoresis — •Alexander Nerowski[1], Markus Pötschke[1], Manfred Bobeth[1], Larysa Baraban[1], Jörg Opitz[1,2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Fraunhofer-Institute for Non-Destructive Testing, 01109 Dresden, Germany

Growth of metal nanowires from solution is a promising "bottom-up" method which can represent an efficient alternative to classical lithography. Here we present a dielectrophoretic growth of nanowires on an amorphous glass substrate in a solution containing Pt-complexes. Aiming at a controlled growth of straight and as thin as possible wires,

the growth process is investigated both in theory and experiment. The metallic nanowire tip is modeled as a sphere electrode. The model includes the dielectrophoretic force on uncharged metal complexes as well as their diffusion in the solution. Experimental data suggest that the deposition process traverses from reaction-limited to diffusion-limited when going from low to high temperatures. Possible reasons for the rate limitation are discussed. Potassium ions in the solution are found to have a great influence on the deposition rate. Finally, we compare the experimentally measured growth velocities with those theoretically calculated.

MM 46.4 Thu 11:00 H 1029

Si/SiO2 nanostructures grown by dewetting of ultrathin amorphous Si-layers for photovoltaic applications — •Jan Amaru Töfflinger[1], Maurizio Roczen[1], Martin Schade[2], Orman Gref[1], Andreas Schöpke[1], Enno Malguth[1], Lars Korte[1], Hartmut Leipner[2], and Bernd Rech[1] — [1]HZB, Inst. Si-Photovoltaik, Berlin, Deutschland — [2]MLU, IZM, Halle, Deutschland

Si nanodots embedded in a SiO2 matrix hold the potential for an enhancement of the efficiency of silicon based solar cells. The application of such Si/SiO2 nanostructures as hetero-emitter on top of an oxidized wafer is investigated. For Si-wafer passivation tunneling oxides with thicknesses down to 1 nm are developed by means of UHV-oxidation using neutral, thermalized oxygen atoms. The density of states at the Si/SiO2 interface as well as its chemical composition is examined via in-situ photoelectron spectroscopy. The UHV-synthesis of Si nanodots is performed by deposition of a thin (1-10 nm) undoped amorphous Si film on top of the oxidized wafer and a subsequent 600°C annealing step. This leads to the self-organized formation of highly crystalline Si nanodots. Nanodot diameters <10 nm are achieved which in principle allows to exploit quantum size effects. The influence of Sb-doping of the initial a-Si film on nanodot formation is investigated. Stacked Si/SiO2 nanodot systems via layer by layer repetition of oxidation and nanodot formation are manufactured and investigated via HRTEM and electrical measurements. Cross sectional images indicate high density of nanodots separated by tunneling oxides allowing an electrical current through the nanodot system by tunneling processes.

MM 46.5 Thu 11:15 H 1029

Tailoring magnetization reversal in magnetic nano-dots with 3D shape modifications — •Tomasz Blachowicz[1] and Andrea Ehrmann[2] — [1]Institute of Physics, Silesian University of Technology, Gliwice, Poland — [2]Hochschule Niederrhein, Faculty of Textile and Clothing Technology, Mönchengladbach, Germany

Understanding reversal mechanisms and dynamics of magnetic nanosystems is one of the leading topics in contemporary physics. In our study, the magnetization reversal dynamics and hysteresis loops of three-dimensional ferromagnetic permalloy half-balls have been examined using micromagnetic simulations and finite element methods [1].

Comparison of samples with different 3D shape modifications enables observations of the nature of switching, oscillation types and frequencies as well as times of reversal, triggered by an external magnetic field. It has been found that a moderate imperfection can enhance the switching process and strongly suppress magnetization oscillations.

Since magnetization characteristics can be modified by changes in the geometry of the magnetic nano-particles, an exact design of the nano-dots allows for tailoring the desired properties for new applications in magneto-electronics, like magnetic field sensors or data storage devices.

[1] T. Blachowicz, A. Ehrmann, P. Steblinski, and L. Pawela: Magnetization reversal in magnetic half-balls influenced by shape perturbations, J. Appl. Phys. 108, 123906 (2010)

MM 46.6 Thu 11:30 H 1029

Electrochemical charging-induced variation of the magnetic moment of γ-Fe_2O_3 nanoparticles investigated by SQUID magnetometry with in-situ cyclic voltammetry — •Stefan Topolovec[1], Peter Jerabek[2], Dorothée Vinga Szabó[3], Heinz Krenn[2], and Roland Würschum[1] — [1]Inst. für Materialphysik, TU Graz, Graz, Austria — [2]Inst. für Physik, Univ. Graz, Graz, Austria — [3]Inst. für Angewandte Materialien - Werkstoffprozesstechnik, KIT, Karlsruhe, Germany

Recently, the reversible variation of the magnetic moment of γ-Fe_2O_3 nanoparticles by electrochemical charging could be demonstrated [1]. In order to study the underlying electrochemical processes in more detail, in-situ cyclic voltammetry in a SQUID magnetometer was performed in the present work. To obtain a conductive electrode, the insulating γ-Fe_2O_3 nanoparticles, which were prepared by microwave plasma synthesis, were intermixed with Pt nanoparticles and compacted to a porous pellet. The magnetic moment of the pellet was measured during recording cyclic voltammograms in a specially designed electrochemical cell. It turns out that the charge dependence of the magnetic moment is significantly affected by reduction and oxidation processes. The magnetic moment could be reversibly tuned up to several percent.

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

[1] T. Traußnig et al., Phys. Status Solidi - Rapid Res. Lett. 5 (2011) 150.

MM 47: Topical Session Modern Atom Probe Tomography III - Functional and Nanostructured Materials

Time: Thursday 10:15–11:45 Location: H 0107

Topical Talk MM 47.1 Thu 10:15 H 0107

Methods in Correlative Tomography for the Nanometer Regime — •Stephan S.A. Gerstl Gerstl, Elisabeth Mueller, Miriam Lucas, and Roger Wepf — EMEZ Center for Electron Microscopy, ETH Zurich, Switzerland

Tomographic methods in materials science have experienced a surge in interest, since observing nature including the third spatial dimension provides significantly more insight than techniques interrogating surfaces or viewing projections of materials. In this paper we discuss a variety of methods we are investigating not only to correlate 3-D images between microscopes, but extend combinatorial techniques to including the correlation between analytical information of chemistry and crystallography. Basic correlations between Atom Probe Tomography (APT) and HRSEM images can reveal geometric input for reconstructions. More direct chemical correlations are feasible between STEM and APT. Methods we will discuss to achieve the spatial and chemical correlations involve modified TEM specimens and well known pillar geometries. Examples from both nanostructured metal and semiconductor type materials will be presented.

MM 47.2 Thu 10:45 H 0107

Laser-assisted atom probe tomography of self-organized surface layers — Andreas Stoffers, Martin Lütkemeier, and •Guido Schmitz — Institut für Materialphysik der Westf. Wilhelms-Universität, Münster, Germany

The availability of femtosecond lasers opened analysis of new material classes by atom probe tomography (APT). Laser-assisted APT has even the potential to give microstructural and chemical information on organic materials at an atomic scale. We investigated the model cases of polyelectrolyte multilayers (PEM) and self-assembling monolayers (SAM). PEMs are deposited step by step as a multilayer of poly-anions and poly-cations to sharp gold tips. SAMs are adsorbed in a self-assembling process to the apex of gold tips, but offer only a limited volume for analysis.

We could successfully analyze multilayers of the polyions poly(acrylic acid), poly(diallyldimethyl-ammonium chloride), poly(styrene sulfonate) and poly(allylamine hydrochloride). Also the chemical structure of perfluorodecanethiol and alcanethiolate SAM was studied. In all cases, mass spectra are complex, indicating different molecular fragments. We could determine the polyanion/polycation stoichiometry in polyelectrolytes, also the amount of counterions. Mass spectra of fluorinated SAM are easily identified. Even the evaporation sequence of molecule fragments could be determined in this case. It appears to be remarkably different to that of structurally similar alcanethiolate monolayers.

MM 47.3 Thu 11:00 H 0107

On the influence of interfaces, local composition and microstructure on the magnetic properties of Nd2Fe14B — •Catharina Wille[1], Torben Boll[1], Tala'at Al-Kassab[1], Manfred Ruehrig[2], and Joachim Wecker[2] — [1]King Abdullah University of Science and Technology, Division of Physical Sciences, Thuwal, Kingdom of Saudi Arabia — [2]Siemens AG, Corporate Research and Technologies, 91058 Erlangen, Germany

In this contribution results on the chemical and microstructural characterisation of a Nd2Fe14B bulk magnet will be reported. As the magnetic coercivity strongly depends on the grain boundary phases, their chemical composition is explored by means of atom probe tomography (APT) in the LAWATAP instrument at King Abdullah University of Science and Technology. Additionally the distribution of Nd in the microstructure and the presence of trace elements like Dy, Ga and Nb has been analysed.

The bulk magnet (MQ2) was prepared by hot pressing from rapidly consolidated powders resulting in an anisotropic microstructure which has been investigated by means of X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS).

Special emphasis was put on the determination of the spatial gradient of the microstructure both parallel and orthogonal to the deformation direction.

MM 47.4 Thu 11:15 H 0107

On the pulse of time: Atom Probe Tomography of nanostructured materials — •Tala'at Al-Kassab, Catharina Wille, and Torben Boll — King Abdullah University of Science and Technology, Division of Physical Sciences,

In the last decade, Nano-materials have been gaining considerable interest for their various properties and applications. Particularly, designed nano-structured materials are largely characterized by their numerous internal interfaces. Since the quested physical properties of this material class are closely related to the thermal stability of their internal interfaces, the investigation of the chemical reactions at these interfaces is of a great importance to understand and optimize the desired properties for prospective future applications. Owing to their grain size of some tens of nanometers, such materials can only be analyzed via high resolution methods such as modern atom probe tomography. This contribution aims at showing by examples, what challenges such atom probe tomographers are able to solve when utilized to explore these nano-structured materials. Results obtained with the laser assisted wide angle tomographic atom probe LAWATAP and the local electrode atom probe LEAP HR4000, which are both newly installed in our laboratory at King Abdullah University KSA, will be presented and compared in this study.

MM 47.5 Thu 11:30 H 0107

Triple junction and grain boundary diffusion in the Ni/Cu system — •Mohammed Reda Chellali, Zoltán Balogh, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms Universität Münster; Münster (Germany)

A topological defect of the grain boundary structure, the so called triple junction, plays a dominant role for grain growth and atomic transport in nano-crystalline materials. By means of atom probe tomography measurement of atomic transport along triple junctions and grain boundaries became possible recently [1]. Heat treatment was chosen in the kinetic C-B regime according to generalized Harrison categories for the hierarchy of volume, grain boundary and triple junction transport. A significant dependence of the thickness of the grain boundaries on the annealing temperature in the range of 563-643 K is detected and taken into account to determine the activation energy along triple junctions. The determined energies are found to be 120 KJ/mol and 82kJ/mol along the grain boundaries and triple junctions respectively. Thus, triple junctions represent a significantly faster diffusion route than grain boundaries.

[1] M-R. Chellali, Z. Balogh, L. Zheng and G. Schmitz Scripta Mater. 65/4 (2011) 343

MM 48: Joint Session Magnetic Shape Memory Alloys I (jointly with DS, MA)

Time: Thursday 10:15–12:00 Location: H 0106

MM 48.1 Thu 10:15 H 0106

Different types of twin boundaries in 14M modulated Ni-Mn-Ga — •Christian Behler[1,2], Bernd Rellinghaus[1], Anja Backen[1], Sandra Kauffmann-Weiss[1], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute for Solid State Physics, Department of Physics, 01062 Dresden, Germany

Recent studies [L. Straka et al. Acta Mat. 59 (2011) 7450-7463] have found that various types of twin boundaries, such as type I, type II and modulation twins, with different mobilities can exist in the magnetic shape memory alloy Ni-Mn-Ga. In a 1.5 μm thin epitaxial Ni-Mn-Ga film we observe two types of twin boundaries. This film was investigated by means of scanning electron microscopy (SEM), transmission electron microscopy (TEM) imaging and selected area diffraction (SAED) to clarify the type of the observed boundaries. From the orientations of neighboring variants, determined by SAED, conclusions can be drawn about the type of the interfaces. These analyzed interfaces can be attributed to type I twin boundaries as well as modulation twins. The 14M modulation is generated by nanotwins, which were observed by High Resolution TEM. However, this modulation is not perfect due to the existence of stacking faults.

MM 48.2 Thu 10:30 H 0106

A multi-phase field model to investigate the elastic and magnetic hysteresis behaviour of twinned Ni_2MnGa — •Marcus Jainta[1], Christian Mennerich[1], Frank Wendler[1], and Britta Nestler[1,2] — [1]IMP, Karlsruhe University of Applied Sciences — [2]IAM-ZBS, Karlsruhe Institute of Technology

In the last years, magnetic shape memory alloys became an important matter for material scientists. Due to their fast response time, their large recoverable strain and the good cost efficiency, this material class is well suited to be used as components of actuators or dampers. The microstructure evolution of magnetic shape memory alloys depends on the formation of magnetic domains and on the elastic strains induced by external magnetic fields and mechanical loads. To represent this behaviour, we applied a multi-phase field model of Allen-Cahn type based on a Helmholtz free energy density formulation. It is coupled with a model for linear elasticity and with an implementation of the Landau-Lifshitz-Gilbert equation. The order parameters are related to the different eigenstrains of the twin variants and to the spontaneous magnetization. In this contribution, we describe the model and compare simulation results of our combined micromagnetic phase-field solver with numerical results from the literature. We present simulation results of twinned structures in martensic Ni_2MnGa performing elastic and magnetic hysteresis behaviours under external forces. We also show the applicability of the model to polycrystalline systems.

MM 48.3 Thu 10:45 H 0106

Modulated martensite and its twin boundaries in Ni-Mn-Ga films — •Anja Backen[1,2], Sandra Kauffmann-Weiss[1,2], Anett Diestel[1,2], Ludwig Schultz[1,2], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute of Materials Science, 01062 Dresden, Germany

The magnetic shape memory alloy Ni-Mn-Ga has gained much attention due to the high achievable strains of up to 10 % when applying an external magnetic field. The reorientation of martensitic variants is achieved by movement of twin boundaries. An external magnetic field can only overcome a twinning stress of 2 MPa or less, which brings the modulated martensite in the center of research interest. The 14-layer modulated martensite exhibits different generations of twin boundaries. The first generation are nano twin boundaries between non-modulated variants which are formed in order to decrease elastic energy at the austenite-martensite interface. The second generation connects variants of the 14M structure. This second generation is highly mobile and can be moved by an external magnetic field. We analyzed two types of microstructures which represent two cases of the 2nd generation of twinning. Although they appear to be completely

different, X-ray diffraction and pole figure measurements reveal that both microstructures are composed of 14M twins. Magnetization measurements show, that only one type of twin boundaries can be moved by a magnetic field which is important for future application in microsystems. This work is funded by DFG via SPP 1239.

MM 48.4 Thu 11:00 H 0106

Freestanding single crystalline Fe-Pd ferromagnetic shape memory membranes: structural, morphological and magnetic characterization — •Yanhong Ma[1], A. Setzer[3], J. W. Gerlach[1], F. Frost[1], P. Esquinazi[3], and S. G. Mayr[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V., 04318 Leipzig — [2]Translationszentrum für Regenerative Medizin und Fakultät für Physik und Geowissenschaften, Universität Leipzig — [3]Faculty of Physics and Earth Sciences, Institute for Experimental Physics II, Division of Superconductivity and Magnetism, Universität Leipzig

Miniaturized single crystalline $Fe_{70}Pd_{30}$ ferromagnetic shape memory alloy membranes in the correct fct phase are synthesized by employing molecular beam epitaxy on MgO (001) substrates at deposition temperatures of 850°C and higher without post-annealing treatment. Atomic force microscopy images of these martensitic Fe-Pd thin films directly reflect formation of twin structure on the surface and reveal, how martensite variants grow. Martensitic phase transformation in the freestanding thin films is investigated with temperature dependent x-ray diffraction and magnetometry using a superconducting quantum interference device. The XRD patterns measured at various temperatures for freestanding martensitic Fe-Pd thin films show reversible (fct-fcc) and irreversible (bcc/bct-fcc) structural transformations.
This project is funded by the Leipzig Graduate School of Natural Sciences "Building with Molecules and Nano Objects" through the German Science Foundation (DFG), as well as by the German Federal Ministry of Education and Research (BMBF, PTJ-BIO, 0313909).

MM 48.5 Thu 11:15 H 0106

Adaptive nanostructures in Fe-Pd magnetic shape memory alloys — •Markus Ernst Gruner[1], Sandra Kauffmann-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

Apart from the prototypical Ni-Mn-Ga Heusler alloy, also Fe-based alloys as $Fe_{70}Pd_{30}$ exhibit significant magnetic field induced strains in moderate magnetic fields. This is bound to a slightly tetragonal fcc structure (fct) which finds no correspondence on the low temperature binding surface which has been determined from density functional theory (DFT) calculations [PRB **83**, 214415 (2011)]. Instead, the energy decreases rather uniformly along the Bain path towards the absolute minimum close to bcc. Recent experiments reveal the possibility of growing $Fe_{70}Pd_{30}$ films with $c/a_{\mathrm{fct}} = 1.09$ extending the Bain path beyond fcc [PRL **107**, 206105 (2011)]. XRD spectroscopy reveals that this is accompanied by a novel relaxation mechanism leading to a nanotwinned pattern consisting of fct building blocks. DFT modelling confirms this process showing a second minimum on the binding surface. This owes to the extremely low formation energy of fct twins causing the autonomous evolution of a twinned superstructure in the simulation cell along [110]. This corresponds to the experimentally observed soft transversal acoustic phonon in this direction, which is also a central feature of the Ni_2MnGa magnetic shape memory alloy. We demonstrate further that magnetic excitations significantly alter the binding surface and thus potentially influence the transformation.

MM 48.6 Thu 11:30 H 0106

Functional properties of magnetic Heusler alloys from an ab initio point of view — •Peter Entel, Mario Siewert, Markus E. Gruner, Heike C. Herper, and Sanjubala Sahoo — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

Magnetic Heusler alloys exhibit complex magnetic phases and multiple intermediate martensitic structures. The strong interplay of magnetic and structural degrees of freedom is decisive for the functional properties associated with the magnetic shape-memory effect and the magneto-, elasto- and barocaloric effect. In this contribution we will discuss how the different functional properties arise from the complex spin interactions between the magnetic ions. We will show that this knowledge can be used to tune and optimize the various functional properties of the Heusler alloys as recently discussed for quaternary magnetic shape memory compounds [1].

[1] M. Siewert *et al.*, Appl. Phys. Lett. **99**, 191904 (2011).

MM 48.7 Thu 11:45 H 0106

Failure of the Maxwell relation for the quantification of caloric effects in ferroic materials — Robert Niemann[1,2], Oleg Heczko[3], Ludwig Schultz[1,2], and •Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Department of Physics, Institute for Solid State Physics, Dresden University of Technology, 01062 Dresden, Germany — [3]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic

Giant caloric effects were reported in elasto-, electro- and magnetocaloric materials near phase transformations. Commonly, their entropy change is indirectly evaluated by a Maxwell relation. We report the fundamental failure of this approach. We analyze exemplarily the Ni-Mn-Ga magnetic shape memory alloy. An applied field results in magnetically induced reorientation of martensitic variants, which form during the phase transformation. This results in a spurious magnetocaloric effect, which only disappears when repeating the measurement a second time. This failure is universal as the vector character of the applied field is not considered in the common scalar evaluation of a Maxwell relation.

MM 49: Nanomaterials II

Time: Thursday 11:45–13:00 Location: H 1029

MM 49.1 Thu 11:45 H 1029

Control of residual less noble element content during dealloying — •Zhen Qi[1] and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany — [2]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Nanoporous metal prepared by the corrosion of an alloy can take the form of monolithic, millimeter-sized bodies containing approximately 10^{15} nanoscale ligaments per cubic millimeter. Applications have been suggested, for instance in catalysis, sensing and actuation. Although the process of dealloying has seen many studies, the underlying processes remain to be clarified in more detail. Here we explore the structure size and residual Ag content in AgAu alloys during electrochemical dealloying. We study different dealloying potentials and a series of alloys including specifically solid solutions that are dilute in Au. A major finding is that nanoporous samples with large content of residual Ag can be prepared. This is surprising in view of the overpotential required for bulk dealloying. The overpotential exceeds the variation of the Ag Nernst potential through the alloy series, suggesting that equilibrium thermodynamics of the bulk alloy alone cannot explain the arrest of the corrosion at finite Ag content. The data set acquired in our study will provide a data base for verifying models of the corrosion process that include capillary terms as well kinetic aspects such as adatom diffusion and vacancy island nucleation.

MM 49.2 Thu 12:00 H 1029

Strengthening of Au-Au bonds in small gold clusters by adsorbing noble gases — •Luca M. Ghiringhelli, Sergey Levchenko, and Matthias Scheffler — Fritz Haber Institute, D-14195, Berlin

In state-of-the-art experiments for the vibrational spectra of metal clusters in the gas phase, photodissociation spectroscopy is performed on clusters complexed with noble gas (RG) atoms, where a RG atom is usually expected to form a weak van der Waals bond. By employing DFT (PBE functional with selected comparisons to PBE0, and to MP2 and CCSD(T) calculations), we surprisingly find a partially covalent bond of *neutral* dimers with RG. For RG = Ar, Kr, Xe one or two RG atoms can bind in a linear molecule with Au_2. While both Hirschfeld and Mulliken analyses show a small electron transfer from the RG to Au_2, the Au-Au bond *shortens* and the Au-Au stretch fre-

quency increases. This is inconsistent with the expected effect of electron transfer to the antibonding orbital of the dimer. Electron-density (n) differences between the bonded systems and the isolated fragments show an accumulation of n between RG and the neighboring Au atom, and between the gold atoms. The analysis of the projected density of states reveals that, although only non-bonding orbital interactions and no charge transfer occurs between RG and Au_2, the d-electrons of Au_2 are redistributed due to the interaction with RG in such a way that the Au-Au σ_s bond is strengthened.

MM 49.3 Thu 12:15 H 1029

Boron Nanotubes: Structural Stability and Electronic Properties — •Viktor Bezugly, Jens Kunstmann, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergman Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

The transport properties, work functions, electronic structure, and structural stability of boron nanotubes with different radii and chiralities are investigated theoretically [1]. As the atomic structure of boron nanotubes and the related sheets is still under debate, three probable structural models are considered. For comparison with recent transport measurements [2], the intrinsic conductance of ideal nanotubes with large diameters is determined. All considered boron nanotubes are highly conductive, irrespective of their lattice structures and chiralities, and they have higher conductivities than carbon nanotubes. Furthermore, the work functions of the three sheets and the corresponding large-diameter nanotubes are determined. It is found that the value of the nanotubes obtained from one model sheet agrees well with the experiment in contrast to the other two models. The energetic stability of nanotubes with diameters >2 nm approaches that of the corresponding boron sheets. However, for smaller diameters the relative stabilities change significantly.

[1] V. Bezugly, J. Kunstmann, B. Grundkoetter-Stock, T. Frauenheim, T. Niehaus, G. Cuniberti, ACS Nano **5**, 4997 (2011).

[2] F. Liu, C. Shen, Z. Su, X. Ding, S. Deng, J. Chen, N. Xu, H. Gao, J. Mater. Chem. **20**, 2197 (2010).

MM 49.4 Thu 12:30 H 1029

Structural and electrical properties of silicon/silicon dioxide nanostructures grown by decomposition of SiOx for photovoltaic applications — •Maurizio Roczen[1], Martin Schade[2], Thomas Barthel[1], Jan Amaru Töfflinger[1], Abdelazize Laades[3], Michael Blech[3], Enno Malguth[1], Hartmut Leipner[2], Lars Korte[1], and Bernd Rech[1] — [1]HZB, Institut für Silizium-Photovoltaik, Berlin, Germany — [2]MLU, IZM, Halle, Germany — [3]CiS, Erfurt, Germany

For the application as nanodot hetero-emitter the self organized growth of Si/SiO2 nanostructures by decomposition of sub-stoichiometric SiOx layers is investigated as well as the structural and electrical and properties of the nanodot system. The SiOx layers are deposited by PVD and CVD techniques onto crystalline Si (c-Si) wafers. The O/Si ratio is obtained by XPS and EDX measurements. XPS shows that decomposition of SiOx is completed after annealing the films at 900 °C. The growth of crystalline Si nanodots is shown in HRTEM images and confirmed by Raman spectroscopy. The size and density of the nanostructures is controlled by the applied annealing temperature and oxygen content. Oxygen rich films show a blue shifted photoluminescence signal which might be related to quantum size effects. Hydrogen concentration of CVD deposited SiOx decreases with increasing oxygen with direct influence on the charge carrier lifetime. The current density through the c-Si/SiOx system decreases with increasing oxygen content. AFM current mapping show a reduction of percolation paths. Doped SiOx induces a band bending of 730 meV in the substrate.

MM 49.5 Thu 12:45 H 1029

Luminescence Properties of Cer-doped Yttrium Aluminum Garnet (YAG:Ce) Nanoparticles - Absolute Quantum Yields and Influence of Particle Size — •Martin Kaiser[1], Christian Würth[1], Ute Resch-Genger[1], Mark Vorsthove[2], and Ullrich Kynast[2] — [1]BAM Federal Institute for Materials Research and Testing, Berlin, Germany — [2]University of Applied Sciences, Münster, Germany

Yttrium aluminum garnet (YAG) doped with Ce3+ (YAG:Ce) is a green-yellow emitting phosphor widely used in the rapidly expanding market of white light LEDs for converting the blue emission of (In,Ga)N-Chips into white. Its advantages compared to other materials include a high photostability and a high luminescence quantum yield (QY) of up to 95 %.

Here, we present measurements of the QY and luminescence lifetimes of a series of YAG:Ce particles of varying sizes ranging from 20 nm to a few micrometer using a new custom designed integrating sphere setup traceably calibrated. The ultimate goal is to understand the influence of the surface-to-volume ratio and the Ce3+ dopant concentration on the photophysical properties of these materials. Our measurements reveal that the QY and decay kinetics are clearly affected by particle size. Low temperature time-resolved measurements were performed to gain a deeper understanding of the decay kinetics.

MM 50: Topical Session Modern Atom Probe Tomography IV - Thin Films and Structural Materials

Time: Thursday 11:45–13:00 Location: H 0107

MM 50.1 Thu 11:45 H 0107

Interface sharpening in miscible Ni/Cu multilayers studied by atom probe tomography — •Zoltán Balogh, Mohammed Reda Chellali, Gerd-Hendrik Greiwe, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms Universität Münster; Münster (Germany)

The chemical analysis of buried interfaces is a delicate task that usually requires well conditioned specimens. The clear and gentle nature of field evaporation and the all 3D subnanometer resolution makes atom probe tomography a method with perspective in this field.

We investigated the effects of diffusional annealing in the miscible Ni/Cu system [1]. We prepared two kinds of samples. The first was produced with abrupt interfaces, while the second type revealed artificially smeared interfaces of about 3 nm in depth. After 15 min annealing at 773 K both types reveal an interface width in between the two different as-prepared values. Thus in the case of the smeared samples, the Ni/Cu interfaces sharpened even though the system is completely miscible at the annealing temperature. Another important observation is that the resulting interfaces were independent of the initial values.

Consequently even though thermodynamic equilibrium predicts infinite continous mixing at the interface, the actual kinetic process, determined by material transport properties, can require nevertheless finite sharpness in intermediate stages.

[1] Z. Balogh, M.R. Chellali, G.-H. Greiwe and Guido Schmitz, Appl. Phys. Lett. 99 (2011) 181902

MM 50.2 Thu 12:00 H 0107

Phase Separation in Immiscible Copper-Tantalum Alloy Films — •Claudia M. Mueller[1], Stephan S.A. Gerstl[2], Alla S. Sologubenko[1], and Ralph Spolenak[1] — [1]Laboratory for Nanometallurgy, Dept. of Materials, ETH Zurich, Switzerland — [2]EMEZ Center for Electron Microscopy, ETH Zurich, Switzerland

Phase separation in binary alloys of immiscible elements is investigated on the copper-tantalum system. The alloys are prepared by co-sputtering followed by annealing to induce phase separation. Local Electrode Atom Probe (LEAP) Tomography in combination with Transmission Electron Microscopy (TEM) and X-ray Diffraction (XRD) is used to study the evolution of phase separation. Results show that in the amorphous copper-tantalum alloys phase separation is coupled to the crystallization of the individual phases. Phase separation starts with the formation of Cu-rich clusters in the still amorphous matrix at temperatures lower than 400°C; the clusters contain up to 10 at% Ta and have a FCC structure with (111) texture. At 600°C the amorphous matrix crystallizes into a β-Ta structure with up to 7 at% Cu dissolved within. It is observed that GBs between Ta nanograins in this sample are enriched with Cu. The amount of Ta that is dissolved in the Cu phase decreases during annealing. The atomic distributions of Cu and Ta in the respective Ta-rich and Cu-rich phases will be discussed in terms of cluster formation and phase growth.

MM 50.3 Thu 12:15 H 0107

Spinodal decomposition in TiAlN/CrN multilayer hardcoatings studied by atom probe tomography — •Ivan Povstugar[1], Pyuck-Pa Choi[1], Jae-Pyoung Ahn[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Korea Institute of Science and Technology, Seoul, Korea

Nanoscale nitride multilayers are good candidates for protective coatings for cutting tools and machine parts owing to excellent mechanical properties and corrosion resistance. However, they possess only a limited thermal stability at operational temperatures. To understand its origin, chemical information at an atomic scale is essentially required. We exploit atom probe tomography to study the thermal evolution of Ti(0.75)Al(0.25)N/CrN multilayers prepared by the sputter deposition.

TiAlN/CrN coating shows well-resolved layered structure with single layer thickness of 4.5 nm. The multilayers are stable up to 600°C when short-range diffusion at layer interfaces begins. At 700°C TiAlN layers undergo interface-directed spinodal decomposition. As a result, each TiAlN layer evolves into a sandwich-like structure consisting of a Ti-rich sublayer confined by two Al-rich ones. With the increase of time or temperature of thermal treatment, the interface-directed mechanism passes into common isotropic spinodal decomposition accompanied by intermixing between TiAlN and CrN layers in a close-to-surface region of the coating. Conversely, Al-rich layers remain clearly distinguishable in the deep region of the coating. The difference is ascribed to the non-uniform release of residual internal stresses during heat treatment.

MM 50.4 Thu 12:30 H 0107

Atom-Probe Tomography of Grain Boundary Oxides in Stressed and Cold-Worked 304 Stainless Steel — •Karen Kruska[1], David W Saxey[2], George D W Smith[1], Takumi Terachi[3], Takuyo Yamada[3], and Sergio Lozano-Perez[1] — [1]University of Oxford, Department of Materials, Parks Road, OX1 3PH, UK — [2]School of Physics, The University of Western Australia, WA 6009, Australia — [3]2Institute of Nuclear Safety System (INSS), 64 Sata, Mihama-cho, Mikata-gun, Fukui 919-1205, Japan

Cold-worked 304 stainless steels (SS) are known to be susceptible to stress corrosion cracking (SCC). This study employs atom-probe tomography (APT) for local chemical analysis of the oxides formed. Autoclave experiments on a set of samples with/without cold-work prior to oxidation, and with/without stress applied during oxidation, were carried out under simulated pressurised water reactor (PWR) primary conditions. APT and analytical transmission electron microscopy (ATEM) were combined to investigate chemical and structural implications of surface and grain boundary oxidation in 304 SS. Focussed ion beam (FIB) milling was used to prepare specimens containing the same grain boundary for every analysis technique. Grain boundary and deformation band oxidation were observed in all but the unstressed and non-cold worked sample. Hydrogen associated to the Nickel-rich regions and cavities was found ahead of the Cr-rich oxide in some of the samples. The implications of these findings to current SCC models will be discussed.

MM 50.5 Thu 12:45 H 0107

The influence of Cu on the microstructure of AlCoCrFeNi high entropy alloys — •Anna Manzoni[1], Nelia Wanderka[1], Sheela Singh[1], Haneen Daoud[2], Rainer Völkl[2], Uwe Glatzel[2], B.S. Murty[3], and John Banhart[1] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Metallische Werkstoffe (Metals and Alloys), University Bayreuth, Bayreuth, Germany — [3]Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

The microstructure of the five element equiatomic AlCoCrFeNi high entropy alloy is compared to the microstructure of six element equiatomic AlCoCrCuFeNi. The influence of Cu on the local microstructure as well as on the local concentration is investigated by SEM, TEM and atom probe tomography. Both as-cast alloys decompose into a dendritic and an interdendritic region. While the six elements alloy shows several Cu-precipitates in both the interdendritic and the dendritic region in addition to Al-Ni and Fe-Cr rich phases, the five elements alloy can be characterized by only two phases both in the dendritic and the interdendritic region. These Al-Ni rich and Fe-Cr rich phases in the AlCoCrFeNi show a very similar composition to those in the AlCoCrCuFeNi alloy. The influence of Cu seems to be limited to the creation of precipitates and to have no influence on the formation of the rest of the microstructure.

MM 51: Computational Materials Modelling VII - Oxides

Time: Thursday 11:45–13:00 Location: TC 006

MM 51.1 Thu 11:45 TC 006

Structural and electronic properties of oxides within a transferable tight binding model — •Alessandro Parma, Georg H. K. Madsen, and Ralf Drautz — ICAMS Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

Using the Tight Binding (TB) approximation charge transfer and magnetism as well as covalent bonding can be modelled. Thereby a TB approximation is obtained by a systematic coarse graining of the density functional theory energy functional. We have implemented an orthogonal pd TB model for transition metal oxides. The optimized minimal basis is obtained by downfolding a multiple-ζ LCAO basis. The bond integrals within the two center approximation are then calculated from a down-folded DFT Hamiltonian. They are found to be continuous and transferable, and allow for a parametrization of the bond energy in terms of exponential functional forms. We use a Stoner model for the inclusion of magnetism and charge transfer is approximated by monopole interactions.

We present the common oxide structures in terms of simple building blocks and analyze them within a close packing approach. Their stability is calculated across the transition metal series and is rationalized in terms of covalent bonding, atomic volume and electronegativity using simple TB models. The Hematite and Wüstite structures are presented in special detail.

MM 51.2 Thu 12:00 TC 006

Molecular Dynamics of Metal Oxide Systems with Polarizable Force Fields — •Philipp Beck[1], Peter Brommer[1,2], Stephen Hocker[3], Johannes Roth[1], Hans-Rainer Trebin[1], and Siegfried Schmauder[3] — [1]Institut für Theoretische und Angewandte Physik (ITAP), Universität Stuttgart — [2]Département de physique, Université de Montréal, QC, Canada — [3]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Universität Stuttgart

Both force field generation and simulation of oxide systems are computationally much more demanding than those of metals or covalent materials due to long-range electrostatic interactions. We used the Wolf [1] direct, pairwise summation method with spherical truncation for Coulomb interactions and extended it to dipolar interactions. The polarizability of oxygen atoms is modeled with the Tangney-Scandalo [2] interaction force field approach. Due to the Wolf summation, the computational effort in simulation scales linearly in the number of particles, despite the presence of electrostatic interactions. Thus, this model allows to perform large-scale molecular dynamics simulations of metal oxides with realistic potentials. In the present contribution, we show the application to several metal oxide systems where simulations of microstructural, thermodynamic and vibrational properties are performed.

[1] D. Wolf *et al.*, J. Chem. Phys. **110**, 8254 (1999).
[2] P. Tangney and S. Scandalo, J. Chem. Phys. **117** 8898 (2002).

MM 51.3 Thu 12:15 TC 006

Thermodynamic stability of Cd_2SnO_4 and Zn_2SnO_4 and their point defects: A comparative study using first-principles methods — •Arno Fey, Péter Ágoston, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstr. 32, 64287 Darmstadt

Ternary oxides represent a possible alternative to current transparent conducting oxides (TCOs). Although high electric conductivities were found for Cd_2SnO_4, the presence of toxic Cadmium in widespread devices is a massive drawback. A possible alternative is Zn_2SnO_4 which is non-toxic and chemically similar, but until now its conductivity is more than one order of magnitude lower. In this study we investigate

both, Cd_2SnO_4 and Zn_2SnO_4, by quantum mechanical calculations within density functional theory (DFT) in order to elucidate the reasons for the different conductivities. We study the thermodynamic stability of various arrangements of the cations in the inverse spinel structure, and the intrinsic point defects as a source for the conductivity. Our results show that Cd_2SnO_4 is thermodynamically stable for certain cation distributions, while no stable phase for Zn_2SnO_4 can be identified. The Sn_{Cd}- and Sn_{Zn}-antisite are the source of the n-type conductivity in these materials.

MM 51.4 Thu 12:30 TC 006

Interplay between defect dipoles and ferroelectric polarization in a lead-free piezoelectric material — •Sabine Körbel and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

$KNbO_3$ is a ferroelectric perovskite-type compound and a special case of the solid-solution system (K,Na)NbO_3 (KNN), which is regarded as a prospective lead-free substitute for today's best material Pb(Zr,Ti)O_3 (PZT) in piezoelectric components. The piezoelectric properties of PZT and KNN are commonly optimized by doping. Depending on the application, ferroelectric hardness or large strain is desirable. Defect dipoles consisting of aliovalent dopants and associated oxygen vacancies can impede domain wall motion and lead to ferroelectric hardening, and in aged ferroelectrics defect dipoles can cause extraordinarily large strains [1]. Combining density-functional theory and classical empirical interatomic potentials, like in [2], we studied defect dipoles consisting of Cu substitutionals and oxygen vacancies in $KNbO_3$. In this way we obtained the energy needed for rotating the ferroelectric polarization around a defect dipole. This energy determines to which extent defect dipoles can pin domain walls, hence contribute to ferroelectric hardening and aging.

[1] X. Ren, Nature Materials 3, 91 - 94 (2004).
[2] S. Körbel and C. Elsässer, Phys. Rev. B 84, 014109.

MM 51.5 Thu 12:45 TC 006

Attracting shallow donors: Hydrogen passivation in (Al,Ga,In)-doped ZnO — •Mozhgan Amini, Masahiko Matsubara, Rolando Saniz, Dirk Lamoen, and Bart Partoens — CMT & EMAT, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium

We show by ab initio calculations that hydrogen passivates the dopant in Al, Ga or In doped ZnO, although hydrogen and (Al, Ga or In) are both shallow donors in ZnO. This puts a limit on the n-type conductivity of the transparent conducting oxide ZnO, in agreement with recent experimental results. Ab initio studies have confirmed the expected attraction between donor and acceptors in ZnO, and between deep and shallow donors in ZnO. Shallow donors, however, are expected to repel each other, as they both donate electrons to the system and become positively charged. But in this work we predict that they can also attract, and, even more important, can form a deep donor level. This is a new passivation mechanism that may also be relevant for other materials.

MM 52: HV Seidman

Time: Thursday 15:00–15:30 Location: H 0107

Invited Talk MM 52.1 Thu 15:00 H 0107

A renaissance in atom-probe tomography for the study of all materials — •David Seidman — Northwestern University, Evanston, Illinois U.S.A.

Atom-probe tomography (APT) is in the midst of a dynamic renaissance because of the of well-engineered instruments, which are robust and ergonomic and capable of collecting large data sets, hundreds of millions of atoms, in short time periods. And additionally the use of data analysis software programs, which are both robust and ergonomic, have dramatically improved the capabilities of APT. The use of picosecond ultraviolet (UV) or green lasers permits one to dissect specimens on an atom-by-atom and atomic-plane by atomic-plane basis at a pulse repetition rate of 1000 kHz. For example, APT is employed to study atomic-scale clustering, the genesis of second-phases, and the microstructural defects that control a metallic alloy's high-temperature mechanical properties. This information provides a detailed understanding on an atomic-scale of the origins of ageing, strength, creep, fracture toughness, corrosion, and irradiation resistance. APT is used to study thin films and multilayers: enabling us to understand them and permits further optimization of, e.g., electronic devices based on thin-films. Laser-assisted APT permits detailed atomic-scale studies of metal-silicide contact formation (silicidation reactions) and phase control, silicon field-effect transistors, and silicon, germanium and GaN nanowires. APT is also used to study organic/inorganic interfaces formed as a result of biomineralization

MM 53: Joint Session Magnetic Shape Memory Alloys II (jointly with DS, MA)

Time: Thursday 15:00–18:45 Location: H 0112

MM 53.1 Thu 15:00 H 0112

Stress accomodation in polytwinned NiTi nanograins studied with the phase-field method — •Christian Mennerich[1], Frank Wendler[1], Marcus Jainta[1], Anna Weisshaar[1], and Britta Nestler[1,2] — [1]Karlsruhe University of Applied Sciences — [2]Karlsruhe Institute of Technology

During the martensitic transformation in NiTi shape memory alloys, grains of a critical radius below about 50 nm do not transform into martensite. A multi-phase field model of Allen-Cahn type is used to analyse the accomodation of a spherical nanograin inclusion embedded in the austenite phase at room temperature. The model is based on a Helmholtz free energy density formulation and includes elastic and eigenstrain energy contributions. The model is implemented using finite differences, assuming staggered grids for the components of the elastic displacements. We present the techniques used to describe the time-spatial evolution of the system oppose this to the simulation of a mechanical equilibrium. The model is successfully applied to Eshelby's inclusion problem to verify the correctness of the implementation. With this model, we study the stress accomodation of polytwinned spherical NiTi nanograins that are embedded in an austenite matrix. The results are compared to analytical solutions and numerical results from the literature.

MM 53.2 Thu 15:15 H 0112

Structure and magnetic properties of epitaxial Fe-Pd-Cu films — •Sandra Kauffmann-Weiss[1], Sven Hamann[2], Markus E. Gruner[3], Peter Entel[3], Ludwig Schultz[1], Alfred Ludwig[2], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden — [2]Ruhr-Universität Bochum, Institut für Werkstoffe, Universitätsstraße 150, 44780 Bochum — [3]University of Duisburg-Essen, Theoretical Physics, Lotharstraße 1, 47048 Duisburg

Epitaxial films are promising candidates for magnetic shape memory (MSM) applications on the microscale. We investigated the magnetic properties of $Fe_{70}Pd_{30-x}Cu_x$ ferromagnetic shape memory alloys with different Cu contents (x = 0, 3, 7) in strained epitaxial films. For the MSM alloy $Fe_{70}Pd_{30}$ we recently demonstrated, that a tetragonal distortion up to 54 % can be induced into the crystal lattice by strained epitaxial film growth [S. Kauffmann-Weiss et al., Phys. Rev. Lett. 107, 2011, 206105]. Due to the tetragonal distortion intrinsic magnetic properties like Curie temperature, saturation magnetisation and magnetocrystalline anisotropy can be controlled. Epitaxial $Fe_{70}Pd_{27}Cu_3$ and $Fe_{70}Pd_{23}Cu_7$ films show slightly lowered values for spontaneous polarisation and Curie temperature, but strongly increased magnetocrystalline anisotropy constants compared to the binary $Fe_{70}Pd_{30}$ alloy and the Ni-Mn-Ga prototype system. These results indicate that alloying of $Fe_{70}Pd_{30}$ with Cu is a promising route to fabricate films with excellent magnetic properties to be used for the MSM effect.

This work is supported by DFG through SPP1239.

MM 53.3 Thu 15:30 H 0112

Dynamic simulation of the giant magnetocaloric effect in Ni-Mn-based Heusler alloys — •Tino Gottschall[1], Jian Liu[1], Konstantin Skokov[1], James David Moore[1], and Oliver Gutfleisch[1,2] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]2Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt, Germany

The origin for the inverse magnetocaloric effect in Ni-Mn-based Heusler alloys is a first-order magnetostructural transition between a low temperature paramagnetic/antiferromagnetic martensite and a high temperature ferromagnetic austenite phase. Performing direct measurements, we report a large adiabatic temperature change ΔT_{ad} exceeding -6 K at a field change of 2 T in a novel Ni-Mn-In-(Co) alloy. Such a giant magnetocaloric effect makes them potential candidates for energy efficient magnetic refrigeration. Far from an ideal first-order transition material, a wide transition temperature range was observed in this sample probably due to the existence of a local inhomogeneity over the sample. The transition distribution has the shape of a Gaussian function. Based on these considerations we were able to simulate the temperature change under adiabatic conditions, which agrees very well with the experimental data. Three parameters to manipulate the dynamic cooling process, namely field dependency, transition width and potential temperature change, are discussed for an in-depth understanding of the underlying physics behind the observed giant magnetocaloric effect.

MM 53.4 Thu 15:45 H 0112

Element-specific temperature dependence of the Ni and Mn magnetization in $Ni_{51.6}Mn_{32.9}Sn_{15.5}$ — •Bernhard Krumme[1], Alexander Auge[2], David Klar[1], Frank Stromberg[1], Andreas Hütten[2], and Heiko Wende[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany — [2]Thin Films and Nanostructures, Department of Physics, University of Bielefeld, D-44801 Bielefeld, Germany

Off-stochiometric compositions of the Heusler compound Ni_2MnSn with an increased content of Mn are known to be ferromagnetic shape memory alloys (FSMA). This class of materials shows a structural phase transition influencing the magnetization as well as the electric resistivity. Therefore, such materials are of interest for applications, e.g. as actuators. We investigated the influence of the structural phase transition on the element-specific magnetization and electronic structure of Ni and Mn in $Ni_{51.6}Mn_{32.9}Sn_{15.5}$ by means of X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD). Due to the element-specificity we were able to reveal a different temperature dependence of the ratio of orbital to spin magnetic moment of Mn compared to Ni. In parallel a change of the electronic structure of Mn is observed, whereas for Ni almost no modifications occur. By applying a magnetic field of 3T in the martensite phase it is possible to reduce the ratio of orbital to spin magnetic moments indicating a field induced reverse martensitic transition (FIRMT).

– Supported by DFG (SFB 491) and SOLEIL, Paris.

MM 53.5 Thu 16:00 H 0112

Effect of the film thickness on the martensitic transformation in Ni-Mn-Sn ultra-thin films — •Niclas Teichert, Alexander Auge, and Andreas Hütten — Department of Physics, Thin Films and Physics of Nanostructures, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld

Off-stoichiometric Ni-Mn-Sn is a ferromagnetic shape memory alloy (FSMA) in certain Mn-rich compositions. The studied alloy shows a phase transformation during cooling from a cubic high temperature austenite phase to a martensite phase with lower symmetry. Subsequent heating leads to the inverse transformation back to austenite. We have produced highly epitaxial $Ni_{51.6}Mn_{32.9}Sn_{15.5}$ thin films of thicknesses between 200 nm and 20 nm on MgO substrates via co-sputtering. The dependency of the martensitic transition on the film thickness was determined by conductivity and anomalous Hall effect (AHE) measurements in the temperature range between 20 K and 340 K. These measurements give us information about the transformation characteristics such as transition temperatures, temperature dependent saturation magnetization and the amount of transforming material for the different films. The AHE is used to analyze the scattering mechanisms during the transformation.

MM 53.6 Thu 16:15 H 0112

Hysteretic aspects of the inverse magnetocaloric effect in martensitic alloys. — Mehmet Acet[1], •Ivan Titov[1], Antoni Planes[2], Lluis Mañosa[2], David González-Alonso[2], and Thorsten Krenke[3] — [1]Fachbereich Physik, Experimentalphysik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]Facultat de Fisica, Departament d'Estructura i Constituents de la Matéria, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Catalonia, Spain — [3]Thyssen Krupp Electrical Steel GmbH, D-4588 1 Gelsenkirchen, Germany

The presence of a large positive entropy change around the martensitic transformation in $Ni_{50}Mn_{35}Sn_{15}$ and in $Ni_{50}Mn_{33.5}In_{16.5}$ is expected to lead to substantial cooling on applying a magnetic field. However, unlike in Ni-Mn-In, the relatively low temperature-shift of the hysteresis with applied field in Ni-Mn-Sn could limit cooling. In both cases we measure direct temperature-change on applying a magnetic field around the reverse and forward branches of the martensitic transition. In Ni-Mn-Sn we initially detect cooling on applying a magnetic field (inverse MCE) and again further cooling on removing the field (conventional MCE). When the field is reapplied once more we detect only warming due to the irreversibility of the metallurgical state of the alloy. In Ni-Mn-In, the temperature change is largely reversible due to the strong shift in the martensitic transformation temperature with applied field. In this case the metallurgical state of the sample can be partially recovered. The results are discussed in relation to the form of the hysteresis and its thermal shift with applied magnetic field.

MM 53.7 Thu 16:30 H 0112

Twin boundaries in trained 10M Ni-Mn-Ga single crystals — •Robert Chulist[1], Alexei Sozinov[2], Ladislav Straka[2,3], Thomas Lippmann[4], Carl-George Oertel[1], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]AdaptaMat Ltd., Yrityspiha 5, Helsinki, FIN-00390, Finland — [3]Laboratory of Engineering Materials, Aalto University, PL 14200, FIN-00076 AALTO, Finland — [4]Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht, D-21502 Geesthacht, Germany

The arrangement of twin boundaries in trained 10M Ni-Mn-Ga single crystals was investigated by electron backscatter diffraction (EBSD) in the scanning electron microscope. Precise monoclinic structure data including direction of modulation were used to determine all possible boundaries. Besides type I, II and compound twins typical for monoclinic symmetry a boundary between two directions of modulation was also detected. Compared to EBSD analysis done with simple tetragonal structure for 10M Ni-Mn-Ga alloys, a more complex microstructure with new boundaries is revealed. The crystallographic results have also been confirmed by diffraction of high-energy synchrotron radiation.

15 min. break

MM 53.8 Thu 17:00 H 0112

Blocking effects of twinning microstructure in Ni_2MnGa thin films — •Tobias Eichhorn, Richard Hausmanns, Peter Klaer, Hans-Joachim Elmers, and Gerhard Jakob — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz

The Heusler compound Ni_2MnGa is one of the rare materials showing a shape memory effect that can be controlled by an external magnetic field. Huge magnetic-field-induced strains (MFIS) of almost 10 % have been demonstrated for bulk single crystals, which makes the compound interesting for actuator applications. Freestanding epitaxial films, as prepared in this work, open up possibilities for miniaturized devices. So far the absence of MFIS in thin film samples at ambient temperature hinders technical implementation. We identify the twinning microstructure, as induced by the film-substrate interaction, to be responsible for blocking effects. The detailed variant configuration and twinning structure for different crystallographic orientation is studied by means of X-ray diffraction and microscopy methods. While (100) oriented samples show an entangled twinning structure, films of (110) orientation possess a promising martensite structure.

Complementary to magnetometry we employ X-ray magnetic circular dichroism measurements to uncover the origin of the magneto-crystalline anisotropy in the system.

This work is part of the DFG priority program SPP 1239.

MM 53.9 Thu 17:15 H 0112

Vibrational properties of Ni-Mn-Ga ferromagnetic shape memory alloys in the austenite phase — •Semih Ener[1], Jür-

gen Neuhaus[1,2], and Winfried Petry[1,2] — [1]Technische Universität München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany

In the ferromagnetic shape memory Ni-Mn-Ga alloys the structural transition can be driven either by an external magnetic field or temperature. In this work we investigate the effect of temperature on the vibrational properties of Ni_2MnGa and $Ni_{49}Mn_{32}Ga_{19}$ in the austenite phase by using mainly inelastic neutron scattering. The measurements were done at the Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching. The Born-von Kármán model is applied to the Ni_2MnGa full phonon dispersion in the austenite phase and macroscopic properties are calculated from this model. The effect of temperature on the phonon softening in TA_2[110] phonon branch is investigated in detail in a wide temperature range for both Ni_2MnGa and $Ni_{49}Mn_{32}Ga_{19}$. The relations between the phonon softening and the structural transition are well understood for both compositions but the effect of magnetic ordering is not comprehended especially for the off-stoichiometric composition.

MM 53.10 Thu 17:30 H 0112

Correlation Between Microstructure and Magnetic Properties in Epitaxial Ni-Mn-Ga Thin Films — •Gesa Welker[1], Aleksej Laptev[1], Mikhail Fonin[1], Yuansu Luo[2], and Konrad Samwer[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen

Ni-Mn-Ga and related alloys exhibit a magnetic shape memory effect and have been subject to research due to their large magnetic field induced strain of up to 10% [1]. So far, only few investigation of their magnetic domain structure has been done on thin films [2].

Here we investigate the morphology and magnetic domain configurations in epitaxial Ni-Mn-Ga thin films grown on MgO(001) substrates by dc-magnetron sputtering [3] as well as in free-standing microstructures released from the rigid substrate by etching. We investigated Ni-Mn-Ga films of different compositions and thicknesses at varying temperatures by means of atomic force microscopy (AFM) and magnetic force microscopy (MFM) in remanence. In the martensitic state we found large domains with out-of-plane magnetization. The domain walls are oriented perpendicular to the martensitic twin boundaries direction. On a smaller scale, the magnetic domain structure is governed by the orientation of the easy axis of the martensitic variants.

Our results could be helpful for the construction of microscale actuators or sensors based on Ni-Mn-Ga thin films.[1] K. Ulakko et al.,Scripta Mater. 36, 1133-1138 (1997)[2] Q. Pan et al., J. Appl. Phys. 91, 7812-7814 (2002)[3] Y. Luo et al., J. Phys. 13, 013042 (2011)

MM 53.11 Thu 17:45 H 0112

Influence of the addition of platinum on the magnetic shape memory alloy Ni_2MnGa — •Mario Siewert, Markus E. Gruner, Heike C. Herper, and Peter Entel — University of Duisburg-Essen, Faculty of Physics

We have studied the influence of the addition of platinum on the magnetic shape memory alloy Ni_2MnGa by means of *ab initio* calculations. In particular, the quaternary system $Ni_{2-x}Pt_xMnGa$ was studied for $0 \leq x \leq 2$. As a main result, the preference of a tetragonal distortion increases with the amount of Pt that is added to the system. The increased preference of the tetragonal $L1_0$-structure goes hand in hand with the onset of antiferromagnetic tendencies in the Pt-rich alloys. The martensitic trends which are observed in the phase diagram of Ni-Mn-Ga are also observed for the alloy systems containing platinum. In particular, the transformation temperature can be further increased when substituting Ga by Mn which introduces additional antiferromagnetic tendencies. The modulated 14M structure which is responsible for the magnetic shape memory effect in Ni_2MnGa, also appears in systems with excess Pt. It turns out that the shape memory effect is about 14% and therefore larger than in Ni_2MnGa.

MM 53.12 Thu 18:00 H 0112

Mapping local elasticity of twinned martensitic NiMnGa films using atomic force acoustic microscopy — •Yuansu Luo[1], Walter Arnold[1,2], and Konrad Samwer[1] — [1]I.Physikalisches Institut, Universität Göttingen — [2]Fachbereich Werkstoffwissenschaften der Universität des Saarlandes, Saarbrücken

Local elasticity of magnetic shape memory films NiMnGa was mapped qualitatively and quantitatively on nanometer scale by means of atomic force acoustic microscopy (AFAM). The films (100nm) used were prepared on MgO substrates by magnetron sputtering. The first bending resonance vibrations of the AFM cantilever were measured by sweeping the frequency from 0.5 to 3MHz. Different contact stiffness was measured in this way for martenstic twin variants due to their anisotropic crystallography. Broad and multi-resonance behavior was observed, reflecting the damping and multi-variant properties of 7-layer modulated martensite. The stiffness image mapped by the measured resonance frequency exhibits however a contrast opposite to the height image mapped by conventional AFM. The result can be associated with the mobility of twin boundaries, namely they are mobile at the top and immobile at bottom of twin lamellas. The load dependent contact indentation was measured. A softening emerges at a critic force and can be contributed to moving of twin boundaries under the local mechanical load. The local elastic moduli were calibrated by a standard sample (SrTiO3). The values evaluated are in the range from 170 to 230 GPa, enlarged by a factor of about 10 compared to stress-free bulk samples. (Supported by BMBF-13N10061)

MM 53.13 Thu 18:15 H 0112

Martensitic and magnetic microstructure of epitaxial Ni-Mn-Ga films — •Anett Diestel[1,2], Anja Backen[1,2], Volker Neu[1], Sandra Kauffmann-Weiss[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

The modulated 14M martensite phase of the magnetic shape memory (MSM) alloy Ni-Mn-Ga shows huge strains up to 10 % by magnetically-induced reorientation of martensitic variants. The interaction between the crystallographic short and the magnetic easy axis is an essential requirement for the MSM effect. For Ni-Mn-a bulk materials a staircase-like domain pattern with 90°- and 180°-domain walls is already known. To understand this interaction in thin films we analyzed the martensitic and magnetic microstructures of epitaxial Ni-Mn-Ga films of different thicknesses by atomic and magnetic force microscopy. The observed domain pattern of thin epitaxial films differs considerably from the bulk concept. Due to the reduced variant width magnetic exchange coupling has to be considered. An interaction between the martensitic microstructure and the magnetic out-of-plane stripe domain pattern was established and a correlation between the domain width periodicity Λ_{DW} and the film thickness d according to $\Lambda_{DW} \sim d^{1/2}$ was identified in good agreement with the theoretical band domain model of Kittel. This work was funded by DFG through SPP 1239.

MM 53.14 Thu 18:30 H 0112

High resolution surface study of modulation in martensites. — •Aleksej Laptev[1], Mikhail Fonin[1], Yuansu Luo[2], Konrad Samwer[2], Emmanouel Pagounis[3], and Markus Laufenberg[3] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen — [3]ETO MAGNETIC GmbH, 78333 Stockach, Germany

In our work we address the preparation of high-quality surfaces of Ni-Mn-Ga single crystals with different stoichiometries as well as of epitaxial Ni-Mn-Ga films [1] and the investigation of their surface structure down to the atomic scale by variable temperature scanning tunneling microscopy (VT-STM) in ultra-high vacuum (UHV) conditions. The (001)-oriented sample surface was studied at different temperatures in both austenitic and martensitic phase. The samples reveal on the nanometer scale in the martensitic state a pronounced surface corrugation which was shown to arise from the modulation in martensites [2]. For off-stoichiometric samples seven- (films) and ten-layered (single crystal) modulation periodicities were found. Atomically resolved pictures reveal atomic rows stacked in sequences with varying periods and occasional stacking faults. On the other hand the stoichiometric single crystal with the 5M modulation shows a very regular modulation periodicity and a different shape of the modulation corrugation. This work was supported by the BMBF-Projects MSM-Sens 13N10061 and 13N10062.

[1] Y. Luo et al., *New J. Phys.* **13**, 013042 (2011).
[2] P. Leicht et al., *New J. Phys.* **13**, 033021 (2011).

MM 54: Computational Materials Modelling VIII - Mechanical Properties and Strain

Time: Thursday 15:45–17:15 Location: TC 006

MM 54.1 Thu 15:45 TC 006

Which alloying element can make tungsten ductile: Insight from density-functional theory — •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, A-8700 Leoben, Austria. — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria.

Based on density-functional theory (DFT), the influence of alloying elements on the $\frac{1}{2}\langle 111\rangle$ screw dislocation in tungsten is investigated to find alloying candidates that make tungsten ductile. The interaction between the alloying atom and the dislocation is calculated by varying the distance between the position of the alloying atom and the center of the dislocation. Positions near the dislocation center turned out to be energetically more favorable for alloying elements with a higher occupation of *d*-electrons. When Mn, Fe, Os or Ir is placed outside the inner most dislocation core, the dislocation starts moving towards this alloying atom. Furthermore, the change of dislocation core symmetry via alloying is determined using both DFT and the inter-row potential approach. A transition from a symmetric to an asymmetric core is revealed for Re, Os, and Ir. Our results implicate that these elements have similar effects on the $\frac{1}{2}\langle 111\rangle$ screw dislocation in tungsten, and therefore, provide atomistic insights to the development of new tungsten materials.

MM 54.2 Thu 16:00 TC 006

How do residual stresses influence the mechanical properties of severly plastically deformed metal composites? — •Tom Marr[1], Jens Freudenberger[2], Alexander Kauffmann[1,2], Hansjörg Klauss[2], and Ludwig Schultz[2] — [1]TU Dresden, Dresden, Germany — [2]IFW Dresden, Dresden, Germany

Severe plastic deformation at room temperature or at temperatures below the recrystallization temperature of various materials is often used to enhance their mechanical properties. By applying these techniques, work hardening is achieved which goes along with a strong grain refinement, texture sharpening and changes in grain boundary characteristics. Residual stresses in these materials are another factor that might contribute to the effective mechanical properties. Surprisingly few works are dealing with this issue despite the fact that especially in composite materials residual stresses are likely to be observed when severe deformation is applied.

In this work, CP titanium, an Al alloy 5049 as well as a composite material made from both materials are cold deformed to logarithmic deformation strains of $\eta = 4$. Tensile tests are carried out on each of them, while finite element calculations are used to simulate the deformation regime of the composite. Finally, a suggestion is given on how residual stresses can act as a contribution to mechanical properties of severely plastically deformed materials on top of cold work, grain refinement, texture development and grain boundary characteristics changes.

MM 54.3 Thu 16:15 TC 006

A canonical stability/elasticity relationship verified for 200.000 face-centered cubic structures — •Sascha B. Maisel, Michaela Höfler, and Stefan Müller — Insitute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

By systematic studies of binary alloy systems via density functional theory and the cluster expansion approach we show that the elastic properties of face-centered cubic intermetallics obey certain rules. Firstly, the stiffness and the heat of formation are negatively correlated with a nearly constant Spearman correlation for all concentrations. Secondly, the probability to find a very stiff structure is negligible in the limit of high enthalpy excess. Lastly, we quantify the probability of finding a meta-stable structure σ harder than the ground-state γ at a specific concentration $x(\sigma) = x(\gamma)$ depending on σ's distance to the ground-state line. The consequences are discussed from both a mathmatical and an application-oriented perspective.

MM 54.4 Thu 16:30 TC 006

Role of coherency strain in the stabilization of metastable precipitate of the Mo-C binary system — •Sankari Sampath, Rebecca Janisch, Suzana G Fries, and Alexander Hartmeier — ICAMS, Bochum, Germany

The precipitation of second phases in metals and metallic alloys is an important phenomenon that has a high influence on the mechanical properties of the material. In a previous computational study, the precipitation behavior of (bct)carbide, MoCx at a grain boundary in Mo(bcc) has been investigated. The study showed that there is a significant strain contribution to the interface energy of the lattice misfit. In the present project, the Mo-C binary system is being studied thoroughly by varying carbon concentrations in the system. The aim is to quantify this strain contribution to the interface energy by means of ab-initio Density Functional Theory using VASP code such that the stabilization of the metastable phase(bct) could be carried out.

The structural stability of various phases of the Mo-C system has been analyzed and compared with experimental results where available.The phase diagram has been obtained using Thermo-Calc and the stable phases agree with our predictions at T=0K. A metastable phase(bct), which is not present in the phase diagram, has been observed experimentally by HREM as a semi-coherent precipitate. We assume that it is stabilized by the precipitate interface energy. Starting with the coherent interface for Mo(001) and MoCx(001),the study has been extended to gamma surface calculations that yield possible Burgers vectors for misfit dislocations.

MM 54.5 Thu 16:45 TC 006

Elastic anomalies and short-range order effects for Ag-Pd alloys — •Martin Hoffmann[1,2], Alberto Marmodoro[3], Eero Nurmi[4], Kalevi Kokko[4], Arthur Ernst[2], and Wolfram Hergert[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Seckendorff-Platz 1, D-06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik,Weinberg 2, D-06120 Halle, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom — [4]Department of Physics and Astronomy, University of Turku, FIN-20014 Turku, Finland

We investigate the elastic properties of the binary alloy Ag-Pd. From the experiment it is known that the lattice constant of this system shows a deviation from the expected linear behaviour according to the Vegard's rule. This was formerly studied by assuming a totally disordered alloy and thereby using the coherent potential approximation (CPA). However, there are predictions of three ordered phases in this system and we include them in our study via supercell calculations. Due to the treatment of certain sub-lattices with the CPA in the Korringa-Kohn-Rostoker formalism we are able to explore the equilibrium properties even in the concentration range between the long-range order structures. We obtain again various deviations from the linear behaviour. As former studies assumed such changes could be observed in concordance with electronic topological transitions in the Fermi surface topology. Using the novel concept of the multi sublattice non-local CPA we introduce short-range order within the same supercell construction.

MM 54.6 Thu 17:00 TC 006

Study of structural anisotropy in Cu50Zr45Al5 metallic glass under uniaxial loading by molecular dynamics simulations — •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 structural anisotropy in Cu50Zr45Al5 metallic glass under uniaxial loading from zero up to 1200 MPa was studied by molecular dynamics simulations. The anelastic strain is found to be negligibly small below 600 MPa whereas it increases with the simulation time from 600 to 1200 MPa. The degree of structural anisotropy and the atomic structure were characterized using a second order fabric tensor and Voronoi tessellation, respectively. Structural analysis indicates that the anelastic deformation occurs via the destruction of clusters with high geometric symmetry. Comparing with our previous results, the degree of anisotropy in Cu50Zr45Al5 MG is about 20-30% lower than that in Cu-Zr MGs under similar loading conditions. It indicates that the covalent bonding around Al atoms tends to stabilize the local structure against anelastic deformation in Cu50Zr45Al5 metallic glass. Finally, the relation between the anelastic strain and shear transformation zones (STZs) is discussed.

MM 55: Topical Session Modern Atom Probe Tomography V - Steels, Alloys and Structural Materials

Time: Thursday 15:45–17:00 Location: H 0107

MM 55.1 Thu 15:45 H 0107

Characterisation by Atom Probe Tomography of a Precipitation Hardened Lean Maraging-TRIP Steel — •Julio Millán, Dirk Ponge, Pyuck-Pa Choi, and Dierk Raabe — Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

Nano-scaled microstructural changes generated in two as-quenched multicomponent alloy systems Fe-xMn-2Ni-1Mo-1Ti-0.15Al-0.01C (x=9 and 12, mass%) during aging at 450°C for 48 hours were evaluated by atom probe tomography. After the solution treatment and subsequent quenching, an initial microstructure consisting of a fully martensite matrix or a mixture of retained austenite and martensite were obtained in the 9%Mn and 12%Mn alloy, respectively. Upon aging, precipitation of nano-sized particles and simultaneous formation of reverted austenite occurred in both materials. No differences in the chemistry of the particles core were found when the nominal Mn content in the alloy was increased from 9 to 12%. However, a difference in formation and growth of the reverted austenite was observed depending on the presence of retained austenite in the quenched state. In absence of retained austenite (9%Mn alloy), the accumulation of Mn together with other alloying elements was detected at the internal interfaces of the martensite matrix, suggesting the formation of a metastable thin-film of reverted austenite. In contrast, the 12% Mn alloy exhibited an accelerated formation of reverted austenite occurring not only at the martensite-martensite interfaces but also around the retained austenite.

MM 55.2 Thu 16:00 H 0107

Analysis of the carbon distribution in a dual phase steel by EBSD and APT — •Lars Schemmann and Stefan Zaefferer — Max-Planck-Institut für Eisenforschung GmbH

Dual phase steels have been invented in the late seventies and early eighties. They combine good mechanical properties, such as a high strength and good formability. Even though they are produced at present time routinely by all big steel companies, some fundamental properties are not perfectly understood. This study focuses on the distribution of carbon in the steel, whereby the gradients at the ferrite martensite border are of special interest. On a microscopic level a combination of EBSD and EDX is used to identify areas of interest. These areas are subsequently analyzed using atomic resolution APT.

MM 55.3 Thu 16:15 H 0107

Atom probe studies on nano-sized precipitates in lightweight steels — •Jaebok Seol[1], Changyung Park[2], Pyuckpa Choi[1], and Dierk Raabe[1] — [1]Max-Planck-Insititut für Eisenforschung, Dusseldorf, Germany — [2]Dept. of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Republic of Korea

Recently, light-weighted steels containing a low Mn of 3 wt.% and a high Al of 6 wt.% have received considerable attention as a new grade of advanced high strength sheet steels (AHSS) due to their excellent combination of strength and ductility.. The mechanical properties of the steel depend on the precipitation of nano-sized (Fe,Mn)3AlC, κ-carbide particles. However, the decomposition of metastable γ (austenite) into α (ferrite) and κ-carbide as a function of isothermal temperatures has not been studied in detail, in particular at the atomic scale. In this work, phase transformation and elemental redistribution within Fe-Mn-Al-C alloys have been studied by electron back-scatter diffraction (EBSD), X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), and atom probe tomography (APT) in conjunction with thermodynamic descriptions. We observe that as austempering temperature increases, the volume fraction of retained γ decreases with increasing the κ-carbide fraction. In addition, APT results reveal the distribution behaviour of alloying elements in the vicinity of α/carbide interfaces. Based on these observations, we evaluate the correlation between the stability of κ-carbide and isothermal temperature.

MM 55.4 Thu 16:30 H 0107

Atom probe tomography analysis of Sr-modified Al-Si hypoeutectic alloy — •Jenifer Barrirero, Michael Engstler, Hisham Aboulfadl, and Frank Mücklich — Functional Materials, Department of Materials Science, Saarland University, D-66123 Saarbrücken, Germany

Al-Si casting alloys are of great industrial importance. The addition of traces of Sr, causes a flake-to-fibrous transition which contributes to the improvement of tensile, impact and thermal shock properties. In order to obtain a better understanding of the underlying mechanisms occurring during this modification, an analysis of Sr distribution was done by laser pulsed atom probe tomography. Site-specific sample preparation of unmodified and modified (150 ppm Sr) hypoeutectic AlSi7 alloy was accomplished by focused ion beam methods. The concentration of Sr at the eutectic Al-Si boundary and its distribution in the eutectic Si were analysed. The results revealed nanometric segregations in the eutectic Si with two to three times more Al than Sr. These features showed linear and planar morphologies which are, to some extent, in agreement with the fundamentals of the impurity induced twinning theory for modification. A morphological comparison between the eutectic Al-Si boundary of modified and unmodified alloys showed a change in the growth front of the eutectic phase as proposed by early theories. The unmodified alloy presented an inhomogeneous jagged boundary in accordance with an endogenous type of growth, while modified specimens had a smoother boundary morphology possibly related to a retarded growth rate of Si.

MM 55.5 Thu 16:45 H 0107

Sr distribution in modified hypoeutectic Al-10Si alloy — •Melanie Timpel[1], Nelia Wanderka[1], Ralf Schlesiger[2], Tomokazu Yamamoto[3], Nikolai Lazarev[4], Dieter Isheim[5], Guido Schmitz[2], Syo Matsumura[3], and John Banhart[1] — [1]Helmholtz-Zentrum Berlin, Berlin, GER — [2]Institut für Materialphysik, Westf. Wilhelms-Universität, Münster, GER — [3]Kyushu University, Fukuoka, JPN — [4]Kharkov Institute of Physics and Technology, Kharkov, UKR — [5]Dep. of Materials Science and Engineering, Northwestern University, Evanston, USA

Small additions of Sr ($\geq$ 200 ppm) to Al-10Si alloy drastically change the morphology of eutectic Si from large plate-like to fine fibrous ('chemical modification'). To understand the mechanisms of modified Si growth the local distribution of Sr in eutectic Si phase has to be clarified. In this study, three-dimensional atom probe tomography and high resolution transmission electron microscopy were applied to locate Sr within the eutectic Si phase. The results of combined investigations indicate local enrichment of Sr (4 at.%) in combination with Al at specific sites of the faceted Si crystal. Linear SrAlSi segregations with tube-like morphology and average width of 4 nm were found at the origin of Si {111} twins, whereas planar SrAlSi segregations with 8×4 nm^2 and length up to 220 nm were found at internal boundaries of eutectic Si. Here we show our results and discuss them with respect to previously postulated modification mechanisms.

MM 56: Biomaterials

Time: Thursday 15:45–16:45 Location: H 0106

MM 56.1 Thu 15:45 H 0106

Performance of biodegradable austenitic Fe-Mn-C-Pd alloys for temporary medical applications — •Michael Schinhammer[1], Isabel Gerber[2], Anja C. Hänzi[1], Jörg F. Löffler[1], and Peter J. Uggowitzer[1] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, Switzerland — [2]Laboraratory for Biologically Oriented Materials, ETH Zurich, Switzerland

Biodegradable metals offer great potential for the use as temporary implant material in vascular intervention and osteosynthesis. They

may overcome some of the restrictions of permanent devices, such as prolonged physical irritation and chronic inflammation. Iron and its alloys are considered promising candidates for such applications. This study focuses on the performance of a biodegradable austenitic Fe-Mn-C-Pd alloy regarding its mechanical properties and in vitro cytocompatibility. The alloys developed feature high ductility values at moderate strength levels and a pronounced hardening, which makes the alloys especially suitable for stent applications. By means of thermo-mechanical treatments the properties can be adjusted over a wide range. In vitro cell testing indicates good cytocompatibility of the eluates, even with increasing eluate concentrations. In summary the property profile of the newly developed alloys appears promising for the use as degradable medical implant material.

MM 56.2 Thu 16:00 H 0106

Influence of the synthetic polypeptide c25-mms6 on Nanoparticle growth — •Annalena Wolff[1], Katrin Wollschläger[2], Katrin Eckstädt[1], Inga Ennen[3], Patrick Thomas[1], Walid Hetaba[3], Stefan Löffler[3], Marco Wissbrock[2], Nadine Mill[1], Thomas Weiss[1], Peter Schattschneider[3], Norbert Sewald[2], and Andreas Hütten[1] — [1]Universität Bielefeld, Fakultät für Physik, Deutschland — [2]Universität Bielefeld, Fakultät für Chemie, Deutschland — [3]Technische Universität Wien, Institut für Festkörperphysik,Österreich

Bioinspired Nanoparticle syntheses have advanced in recent years. Polypeptides play a key role in the controlled biomineralization process. Their influence on inorganic crystal growth has not yet been understood. A bioinspired synthesis of Cobalt Ferrite nanoparticles was carried out in vitro at room temperature. Here a short synthetic version of the protein MMS6, found to be involved in the biomineralization process within Magnetotactic Bacteria was used to synthesize the magnetic nanoparticles. The influence of this synthetic polypeptide was studied by comparing the obtained Cobalt Ferrite Nanoparticles to those synthesized without polypeptide. Stoichiometric Cobalt Ferrite Nanoparticles were obtained in the polypeptide enhanced synthesis while non-stoichiometric Cobalt Ferrite nanoparticles were found in the control experiment. Our results indicate that the polypeptide influences the microstructure but is not required to obtain particles. On the basis of our results we propose a multistep biomineralization process in which the polypeptide acts as a catalyst.

MM 56.3 Thu 16:15 H 0106

On the role of Mg atoms in calcite crystals: an *ab initio* study — •Pavlína Elstnerová[1], Martin Friák[1], Tilmann Hickel[1], Helge Otto Fabritius[1], Dierk Raabe[1], Andreas Ziegler[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]University of Ulm, Ulm, Germany

Nearly 90% of animal species protect themselves with a cuticle: a complex hierarchical biocomposite often containing calcite that acts as a stiffening component. These calcite crystals contain impurities, commonly Mg or P, but the role of these elements is much debated. Here we present results of a parameter-free quantum-mechanical study of the thermodynamic, structural and elastic properties of single calcite crystals containing Mg atoms employing density functional theory (DFT). We calculated the electronic structure of bulk $(Ca_xMg_{x-1})CO_3$ using 30-atomic supercells and studied the impact of Mg substitutions. Our calculations show that replacing Ca by Mg reduces the volume of substituted crystals and increases their bulk modulus as well as uniaxial and biaxial Young's moduli. Our results thus indicate that the role of Mg in calcite crystals is to stiffen the material (for details see Elstnerová *et al.*, *Acta Biomater.* **6** (2010) 4506). We also find significant Mg-induced local distortions of lattice geometries (involving carbonate groups) that are similar to those found at calcite surfaces.

MM 56.4 Thu 16:30 H 0106

How to detect protein fouling and cleaning in heat exchangers using ultrasonic based measurements and classification methods — •Eva Wallhäusser, Mohamed Hussein, and Thomas Becker — TU München. Brau- und Getränketechnologie, (Bio-)Prozesstechnik und Prozessanalyse, Weihenstephaner Steig 21, 85354 Freising

Fouling and cleaning are severe issues in industries using heat exchangers. In particular food and pharmaceutical industry is concerned. Due to fouling unsupervised cleaning takes place which leads to high production costs. A setup was developed to produce and measure dairy protein fouling under realistic conditions. This setup was characterised theoretical using wave equations, port theory, and sensitivity analysis. Also, experimental validation was done. Dairy protein fouling was produced under flow conditions and it was shown that it is possible to detect its presence and absence using an ultrasonic measuring method. For this, an algorithm was developed which is based on a combination of acoustic and signal parameters which are fed into classification methods like artificial neural network (ANN) and support vector machine (SVM). Offline, detection accuracy of the ANN was 97.80 % and of the SVM 97.38 %. The code was then adapted and implemented for online analysis using an ANN as classification method. First online tests for cleaning succes were done.

MM 57: Complex Materials I

Time: Thursday 15:45–17:00 Location: H 1029

MM 57.1 Thu 15:45 H 1029

Quasikristalle - Clusterkristalle mit Defekten — •Hartwig Schlüter — SCHLÜTER CONSULT, Maschmühlenweg 8-10, 37073 Göttingen

Anders als bisher angenommen, kann eine dichteste Atom-/Kugelgelpackung aus Clustern mit ikosaedricher Symmetrie erzeugt werden. Bausteine sind ein Bergman-Cluster mit 20 Kugeln in der äußeren Schale und ein Mackay-Cluster mit 30 Kugeln auf den 2f-Symmetrieachsen der äußeren Clusterschale. Bei dem Mackaytyp-Cluster 2. Generation(2. Gen.) befinden sich die Bergman-Cluster 1. Gen. auf den Schalen mit geradzahligem Schalenindex und die Mackay-Cluster 1. Gen auf den Schalen mit ungeradem Schalenindex - oder umgekehrt. Nächstenachbar(NN)-Cluster 1. Gen. aus NN-Schalen besitzen 5 Koinzidenzplätze. NN-Bergman-Cluster 1. Gen. besitzen 2 Koinzidenzplätze und NN-Mackay-Cluster 1. Gen. besitzen 4 Koinzidenzplätze. Aus geeigneten Clustern 2. Gen. wird ein Cluster 3. Gen. konstruiert, der aus 20 "Cluster-Einkristallen"besteht. Dieses Strukturmodell erlaubt es, Quasikristalle mit ikosaedrischer Symmetrie als Kristalle mit Defekten zu beschreiben.[1]

[1] Models of the Atomc Structure of Approximants and related Quasicrystals, Hartwig Schlüter, SCHLÜTER CONSULT, Göttingen, 2011 (www.schlueter-consult.de)

MM 57.2 Thu 16:00 H 1029

Studying plastic deformation in brittle complex metal alloys: deformation of Al13Co4 at room temperature — •Sandra Korte[1,2], Volker Schnabel[2], and William J Clegg[2] — [1]Friedrich Alexander Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]University of Cambridge, Cambridge, UK

In this paper the low temperature deformation behaviour of single crystals of orthorhombic Al13Co4 has been studied using micropillar compression. This technique allows the study of plasticity by suppressing cracking in brittle materials as the sample size is reduced to a few microns. Therefore, a polycrystal of sufficient grain size allows the milling of micropillars as single crystalline samples and the selection of different crystal orientations by correlation with electron backscattered diffraction. The plastic deformation of such small single crystals has been studied in terms of the stresses involved and structures observed by scanning and transmission electron microscopy after deformation. It was found that features correlating to crystallographic slip on the glide planes expected based on experiments at higher temperatures mainly occurred where these were oriented favourably, with a high resolved shear stress. In other orientations deformation bands were observed to form on planes of maximum shear stress. This is discussed in the light of the deformation morphology, strain-rate dependence and similar deformation signatures found in bulk metallic glasses.

MM 57.3 Thu 16:15 H 1029

Quantum Diffusion in Metallic-Mean Labyrinth Tilings — •Stefanie Thiem and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

We present results for the quantum diffusion in quasiperiodic tight-

binding models in one, two, and three dimensions. The models are based on a class of one-dimensional quasiperiodic chains, in which the atoms are coupled by weak and strong bonds aligned according to the metallic-mean sequences. The associated labyrinth tilings in d dimensions are then constructed from the direct product of d such chains, which allows us to consider rather large systems numerically. The electronic transport properties are studied by computing the scaling behavior of the return probability and the mean square displacement of wave packets with respect to time. Our results reveal that the systems exhibit anomalous diffusion, where this behavior can be related to the underlying quasiperiodic structure by applying a renormalization group approach and perturbation theory.

MM 57.4 Thu 16:30 H 1029

Role of phason fluctuations for the stability of a quasicrystal model system — •Alexander Kiselev[1], Michael Engel[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Department of Chemical Engineering, University of Michigan, USA

The source of stability of quasicrystals is generally not well understood. A common model assumes that structural fluctuations, which are not present in periodic approximant crystal structures, play an important role by contributing a configurational term to the free energy. Here, we study the influence of phason fluctuations on the stability of a decagonal quasicrystalline model system, where the atoms interact by the Lennard-Jones-Gauss potential [1], and apply molecular dynamics and Monte Carlo simulations. Absolute values of the Free energy were calculated by the Frenkel-Ladd method [2] for the phononic part and by the phason flips decoupling approach for the configurational part. A phase transition from an energetically stabilized periodic Xi-approximant to an entropically stabilized random tiling quasicrystal is observed. We simultaneously have observed the phason elastic constants. One phason elastic constant changes its sign from positive to negative when the temperature at the Xi-quasicrystal transition is lowered, indicating a soft-phason transition.

[1] M. Engel and H.-R. Trebin, Phys. Rev. Lett. **98** 225505 (2007)
[2] D. Frenkel and A.J.C. Ladd, J. Chem. Phys. **81** 3188-3193 (1984)

MM 57.5 Thu 16:45 H 1029

Defects in the monoclinic Al-Pd-Fe complex metallic alloy — •Michael Feuerbacher and Marc Heggen — Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The complex metallic alloy phase m-Al-Pd-Fe, a ternary extension of the Al13Fe4 phase, has a monoclinic structure (space group C1 2/m, lattice constants a = 1.55 nm, b = 0.88 nm, c = 1.25 nm). The unit cell contains 102 atoms, which are coordinated in the form of icosahedral clusters.

We present a characterization of defects in as grown and plastically deformed m-Al-Pd-Fe by means of aberration-corrected high-resolution scanning transmission electron microscopy using a high-angle annular dark-field detector. In the deformed samples we find dislocations trailing stacking faults at a high density, which mediate plastic deformation in the structure. We identify the displacement vectors of the stacking faults and the dislocation Burgers vectors. We demonstrate that the dislocations are metadislocations and discuss their relation to metadislocations in orthorhombic Taylor phases.

MM 58: Topical Session Modern Atom Probe Tomography VI - Ordering, Clustering and Segregation

Time: Thursday 17:00–18:00 Location: H 0107

MM 58.1 Thu 17:00 H 0107

Atom Probe Tomography Analysis of Local Chemistry Fluctuations in Fe-based Alloys Affecting Bulk Deformation Behaviour — •Ross Marceau, Pyuck-Pa Choi, and Dierk Raabe — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The solute architecture within an alloy solid solution is increasingly recognised as a key factor in engineering the evolution of microstructure. Improved performance of advanced materials requires better understanding of how the structure and chemistry at the nanometre scale impact the overall properties, however the challenge is that characterising atomistic-level structures pushes the limits of resolution and detection of most microscopy techniques. Atom probe tomography (APT) provides a unique combination of highly resolved atomistic information, both chemically and spatially in three dimensions, which can be data-mined for quantitative nanostructural information that can be seeded directly into computer simulations to predict bulk material properties of industrially significant materials.

This project is designed in the context of high-Mn TWIP steel and a model Fe-Al intermetallic alloy, where the aim of this work is to quantitatively identify fluctuations in local chemistry using state-of-the-art analysis techniques to discern fine-scale atomic clustering/segregation phenomena. These fluctuations in local composition include short-range ordering (SRO); reputed to affect the local stacking-fault energy (SFE) of the material and thus also local and global deformation pathways.

MM 58.2 Thu 17:15 H 0107

Short range order and its correlation with anti phase boundaries in Ni2(Cr0.5,Mo0.5) alloy — Amit Verma[1,2], •Nelia Wanderka[1], Nikolai Lazarev[3], J.B. Singh[2], and M. Sundararaman[4] — [1]Helmholtz Zentrum Berlin, Berlin, Germany — [2]Mechanical Metallurgy Division, Bhabha Atomic Research Centre, Mumbai, India — [3]NSC Kharkov Institute of Physics and Technology, Kharkov, Ukraine — [4]Hyderabad Central University, India

Nickel base Ni2M (M = Cr, Mo, V, W) alloys belong to {1 1/2 0} family of alloys which undergo disorder to order transformation via a short-range order (SRO) state. In the present work, SRO to LRO transformation has been investigated in the alloy with solution treated initial microstructure. The ordering sequence has been studied using resistivity measurements and the change in resistance is correlated with microstructure. Atom probe (3D-AP) investigations revealed the presence of composition fluctuations of N2M2, N3M, N4M type (where N represents Ni atom and M represents Cr and Mo atoms). Transmission electron microscopy investigations carried out on fully ordered samples revealed the presence of anti-phase boundaries (APBs) which contained N2M2 type compositional clusters as established by TAP investigations. The appearance of the SRO state during the dissolution of the LRO could thus be attributed to the N2M2 clusters at APBs as revealed by resistivity investigation.

MM 58.3 Thu 17:30 H 0107

Atom probe tomography study of the clustering and crystallization kinetics in FeSiNbBCu alloys — •Pradeep Konda Gokuldoss[1], Pyuck Pa Choi[1], Aleksander Kostka[1], Stefanie Sandloebes[1], Dierk Raabe[1], and Giselher Herzer[2] — [1]Max planck Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — [2]Vacuumschmelze GmbH & Co. KG, Hanau, Germany

Partially nanocrystalline FeSiNbBCu alloys with about 25 vol. % retained amorphous matrix are used for their excellent soft magnetic properties. Rapidly solidified Fe-Si-Nb-B-Cu amorphous ribbons upon annealing undergo nanocrystallization, where soft magnetic Fe-Si nanocrystals are formed. Nanocrystallization of Fe-Si grains in these compounds is kinetically governed by the size and density of Cu clusters that precede Fe-Si crystallization. In this work we study the kinetics of Cu clustering and subsequent Fe-Si nano-crystallization in an amorphous Fe73.5Si15.5Cu1Nb3B7 alloy, by atom probe tomography. The microstructural changes in terms of the number density of Cu clusters and the resulting size difference of Fe-Si nano crystals during isothermal and isochronal kinetic studies will be presented. Also, the direct implications of these microstructural changes on the soft magnetic properties will be discussed.

MM 58.4 Thu 17:45 H 0107

Decomposition and ordering in Ni-11.3 at.% Ti as studied by Atom Probe Tomography — •Tala'at Al-Kassab[1], Torben Boll[1], Catharina Wille[1], and Bernd Schönfeld[2] — [1]King Abdullah University of Science and Technology, Division of Physical Sciences, — [2]Laboratory of Metal Physics and Technology, Department

of Materials, ETH Zurich,

Recent results obtained on the decomposition path in Ni-rich Ni-Ti are reported. For this metallic system, there are different reports with respect to the decomposition path at elevated temperatures (around 873 K). As atom probe tomographers are now collecting data in a comparatively large volume, more detailed information may now be deduced, in particular, on the early stages of decomposition. For this study single crystals of Ni-11.3 at.% Ti were grown by the Bridgman technique. Platelets were homogenized at 1443 K, quenched into brine and aged at 873 K for 5, 23, 95 and 219 h, respectively. Tips were then prepared with a <100> axis. Atom Probe Tomography analysis was performed with a position sensitive detection system, named LAWATAP at the newly established Laboratory at King Abdullah University of Science and Technology. The composition of the precipitates and the existence of aging stages will be discussed.

MM 59: Complex Materials II

Time: Thursday 17:00–18:15 Location: H 1029

MM 59.1 Thu 17:00 H 1029

An atomic model for Metadislocation Motion: How do hundreds of Atoms move in a coordinated way? — •Marc Heggen and Michael Feuerbacher — Peter Grünberg Institut, Forschungszentrum Juelich GmbH, D-52425 Juelich

Metadislocations are highly complex defects which involve several hundreds of atoms in their core. We present a microstructural investigation on Metadislocations in the complex metallic alloy xi'-Al-Pd-Mn using aberration-corrected high-resolution scanning transmission electron microscopy. We show that the metadislocation core is highly ordered and based on atomic clusters. It possesses a multiscale structure with an inner core comprising the full strain of the metadislocation and an outer core which is not strained but has a modified cluster structure with respect to the bulk. A first atomic model for metadislocation motion is presented which involves the coordinated movement of hundreds of atoms along various directions.

MM 59.2 Thu 17:15 H 1029

Magnetic and transport studies on Ce(Pd1-xCux)3 alloys — •Mahboubeh Houshiar — Shahid Beheshti University, Tehran, Iran

The system of compounds Ce(Pd1-xCux)3 with (x = 0, 0.017, 0.033 and 0.133) crystallize in the cubic AuCu3 - type structure with copper entering the lattice in substitution for Pd. With increasing copper content they show temperature shifts in max resistivity and TEPmax, but for higher concentration the maximum disappears. The susceptibility shows a large reduction in the paramagnetic Curie temperature with increasing x which indicate rapid decrease of the Kondo temperature with increasing copper content.

MM 59.3 Thu 17:30 H 1029

Pinning of Domain Walls in Helical Magnets — •Bahman Roostaei and Thomas Nattermann — Institute for Theoretical Physics, University of Cologne, Cologne , Germany

Helical magnets are realized in frustrated antiferromagnets, e.g. in rare earth metals Er, Tb, Dy, and Ho or as well in alloys like Gd_xY_{1-x} and $CsCuCl_3$. In centro-symmetric crystals the helical order may be left or right handed. It was shown recently that helical magnets exhibit a new type of domain walls which includes vortex lines. We have developed a theory for these domain walls that can address their static and dynamic properties based on basic microscopic parameters of the system. In particular we have calculated the elastic constants of such vortex walls and tested our theory numerically. One of the most important questions about domain walls in helical magnets is their interaction with disorder present in the system. We have investigated the effect of disorder on the roughness of these walls. Normally, in the presence of disorder there is a finite threshold force density for depinning the wall. we have modeled the near-threshold dynamics of the vorex walls and estimated the threshold force based on vortex properties and other microscopic parameters of the system.

MM 59.4 Thu 17:45 H 1029

Thermal stability and soft magnetic properties of Co-Fe-Hf-B glassy alloy with wide supercooled liquid region — •Amir Hossein Taghvaei[1,2], Mihai Stoica[1], Uta Kühn[1], and Jürgen Eckert[1] — [1]IFW Dresden, Germany — [2]Shiraz University, Shiraz, Iran

A new glassy alloy with composition of Co40Fe22Hf6.5B31.5 was synthesized by melt spinning method. The thermal stability and crystallization process were investigated by differential scanning calorimetry (DSC) and X-Ray diffraction (XRD) in reflection mode using Co Kα radiation. The DSC profile of ribbons showed the glass transition at 903 K, followed by a supercooled liquid region of 62 K before crystallization. The glassy phase devitrified through a single sharp exothermic peak in to (Co, Fe)2B, (Co, Fe)3HfB2 and (Co, Fe)21Hf2B6 intermetallic compounds. The activation crystallization energy of 912 KJ/mole measured using the Kissinger approach, confirmed the very high thermal stability of this alloy. Magnetic measurements indicated that the as cast ribbon has the coercivity, magnetization and Curie temperature of 5 A/m, 47 Am2/kg and 431 K, respectively.The high thermal stability can be explained by the sluggish nucleation and slow growth of the complex (Co, Fe)3HfB2 and (Co, Fe)21Hf2B6 intermetallics.

MM 59.5 Thu 18:00 H 1029

Crowding phenomenon of scattered probe atoms in a Supercooled binary Lennard-Jones mixture — •Imad Ladadwa[1] and Andreas Heuer[2] — [1]FBSU, 15700 Tabuk, KSA — [2]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstrasse 30, 48149 Münster, Germany

The crowding effect phenomena have been investigated by performing a molecular dynamics simulation on a three dimensional Lennard-Jones binary mixture. When coupling a small randomly chosen fraction of particles to an external field we observed that these particles tend to form strings. Their sizes strongly depend on the external driving force as well as on the simulation time. This behaviour reflects a crowding effect which resembles an induced effective attraction force acts on the probe atoms and drives them to create a string like structures. The formation of these strings as a collective cooperative motion leads to a significant modification of the non-linear behavior of the velocity-force relation.

MM 60: Computational Materials Modelling IX - Interfaces and Boundaries

Time: Thursday 17:15–19:00 Location: TC 006

MM 60.1 Thu 17:15 TC 006

Atomistic modelling of interfaces between cubic phases and complex phases in refractory metals — •Thomas Hammerschmidt, Miroslav Cak, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Topologically close-packed (TCP) phases play in important role in many modern alloys and steels. The TCP phase stability can be attributed to an interplay of bandfilling effects and differences in atomic size. In order to shed light on the precipitation of TCP phases, we study their interfaces to cubic phases. Here, we have chosen the interfaces bcc-A15 and fcc-σ due to their technological relevance in W thin films and in Ni-based superalloys, respectively. We investigate the interface formation energy by atomistic simulations with electronic structure methods at different levels of coarse-graining. On the tight-binding level, we employ simple canonical models to investigate relations between band-filling and interface structure. On the level of bond-order potentials (BOP), an approximation to the tight-binding scheme, we employ recently developed parametrisations for refractory metals. With the analytic BOPs we observe that the interface energy

of a commensurate interface of multiple unit cells is minimised by a coincidence-site-lattice arrangement. We then minimise the interface energy with respect to the number of atoms by directly employing the atom-resolved binding energies of the analytic BOP. Our observation of a more densely packed interface for increased bandfilling can be attributed to a decrease in the covalent character of the bonds.

MM 60.2 Thu 17:30 TC 006

The stability of Bi-Te and Sb-Te layered structures: a first-principles study — •Kirsten Govaerts[1], Marcel H.F. Sluiter[2], Bart Partoens[3], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Department of Materials Science and Engineering, 3mE, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands — [3]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Using an effective one-dimensional cluster expansion in combination with first-principles electronic structure calculations we have studied the energetics and electronic properties of Bi-Te and Sb-Te layered systems. In order to get a fast convergence we used a (pseudo)ternary cluster expansion, which takes into account the formation of Sb or Bi bilayers after relaxation due to a Peierls distortion of the lattice. With this new method, groundstates of Bi-Te and Sb-Te can be found without making the dataset of ab initio calculated structures unreasonably large. For a Te concentration between 0 and 60 at.% an almost continuous series of (meta)stable structures is obtained consisting of consecutive X bilayers next to consecutive X_2Te_3 units, with X corresponding to Bi or Sb. Our calculations (at T = 0 K) do not show evidence for the existence of separate single phase regions. Metastable compounds with a Te concentration between 0 and 40 at.% are semimetallic, whereas compounds $(X_2)_n(X_2Te_3)_m$ $(n, m = 1, 2, ...)$ with a Te concentration between 50 and 60 at.% are semiconducting. Compounds with an odd number of consecutive X layers are metallic.

MM 60.3 Thu 17:45 TC 006

Interfaces of hybrid materials: Structure and properties of silylated TiO_2 surfaces — •Beatrix Elsner, Wolfgang Heckel, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

Silane coupling agents are commonly used to modify the interface properties of composite materials such as ceramic-polymer systems. The ability to control the interface stability is a key to modern materials design. Using density functional theory, we have investigated the adsorption characteristics of silane coupling agents on the low-index surfaces of rutile titanium dioxide. The resulting energetics are strongly linked to surface stability and adsorption geometry. We found that the less stable surfaces allow for higher coupling agent coverage as they contribute more dangling bonds to the adsorbate. Further the divergency from ideal silicon tetrahedral angles displays a strong influence on the binding energy. Hence a detailed knowledge of the atomic structure is crucial to understand the interface properties of hybrid systems.

MM 60.4 Thu 18:00 TC 006

Simulations of grain boundary migration via the nucleation and growth of islands — •Christopher Race, Johann von Pezold, and Joerg Neugebauer — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Deutschland

Classical molecular dynamics simulations of bicrystals have been much used to explore the motion of grain boundaries. Commonly, previous studies were designed to explore the large configurational space of possible grain boundary structures and so necessarily employed small simulation cells. In such small cells the whole area of the grain boundary is constrained to move simultaneously and so the boundary remains atomically flat. The formation of important features such as double kinks and islands is often absent.

We have therefore studied the motion of a symmetric tilt boundary in system sizes large enough to accommodate the nucleation and growth of stable islands of migrated crystal volume. We consider the effect of the driving force for grain boundary motion on the size of a critical island nucleus and on the energy barrier for its formation. Based on our results we identify two distinct regimes of mesoscale migration mechanism (island-based vs. flat) in terms of driving force and system size. We consider the implications of this insight for the interpretation of results of typical grain boundary simulations.

MM 60.5 Thu 18:15 TC 006

Hydrogen diffusion in Fe grain boundaries: A kinetic Monte Carlo study — •Yaojun A. Du[1], Jutta Rogal[2], and Ralf Drautz[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany — [2]ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Hydrogen embrittlement in iron and steels is a complex problem that is still not fully understood. Structural defects in the material such as vacancies, grain boundaries, and dislocations can trap hydrogen and a local accumulation of hydrogen at these defects can lead to a degradation of the materials properties. An important aspect in obtaining insight into hydrogen embrittlement on the atomistic level is to understand the diffusion of hydrogen in these materials.

In our study we employ kinetic Monte Carlo (kMC) simulations to investigate hydrogen diffusion in bcc iron including the effect of different microstructures. All input data to the kMC model, such as available sites, solution energies, and diffusion barriers are based on *ab initio* calculations. In particular we consider an idealised cubic grain structure exhibiting bulk and interface sites, an idealised layered structure and a more realistic model of the $\Sigma5[001](310)$ grain boundary in bcc-Fe. We find that hydrogen mainly diffuses within the interface region with an overall diffusivity that is lower than in pure bcc-Fe bulk. To describe the macroscopic diffusion behaviour we derive an analytic expression as a function of hydrogen concentration and temperature which is in excellent agreement with our numerical results.

MM 60.6 Thu 18:30 TC 006

Interfacial layering of a room-temperature ionic liquid thin film on mica surfaces — •Daniele Dragoni[1], Nicola Manini[2], and Pietro Ballone[3] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne — [2]Dipartimento di Fisica, Universitá degli Studi di Milano — [3]Atomistic Simulation Centre, Queen's University Belfast.

We investigate the structure of a thin (4 nm) [bmim][Tf_2N] film on mica by molecular-dynamics simulations using an empirical force field. Interfacial layering at $T = 300$ K and at $T = 350$ K is investigated by determining the number- and charge-density profiles of [bmim][Tf_2N] as a function of distance from mica, and by computing the normal force F_z opposing the penetration of the ionic liquid film by a hard nanometric tip, represented by a spherical particle interacting with [bmim][Tf_2N] atoms by a short range potential. The results show that layering is important but localized within ~ 1 nm from the interface. The addition of a surface charge on mica, globally neutralised by an opposite charge on the [bmim][Tf_2N] side, gives rise to low-amplitude charge oscillations extending through the entire film. However, outside a narrow interfacial region, the resistance of the [bmim][Tf_2N] film to penetration by the mesoscopic tip is only marginally affected by the charge at the interface. The results obtained here for [bmim][Tf_2N]/mica are similar to those obtained using the same method for the [bmim][Tf_2N]/silica interface, and agree reasonably well with experimental force-distance profiles measured on this last interface at ambient conditions.

MM 60.7 Thu 18:45 TC 006

Dispersive and Covalent Interactions Between Graphene and Metal Surfaces from the random phase approximation — •Thomas Olsen — Technical University of Denmark

The potential energy surfaces for graphene adsorbed on Cu(111), Ni(111), and Co(0001) have been calculated using density functional theory and the Random Phase approximation (RPA) (PRL 107 156401). For these adsorption systems covalent and dispersive interactions are equally important and while commonly used approximations for exchange-correlation functionals give inadequate descriptions of either van der Waals or chemical bonds, RPA accounts accurately for both. It is found that the adsorption is a delicate competition between a weak chemisorption minimum close to the surface and a physisorption minimum further from the surface.