MM 17: Postersession I

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

MM 17.1 Mon 18:00 Poster E

Microstructural characterization of hydrogen induced cracking in TRIP-assisted steels by EBSD — •Aurélie Laureys, Tom Depover, Roumen Petrov, and Kim Verbeken — Department of Materials Science and Engineering, Ghent University (UGent), Technologieparkt 903, B-9052 Ghent, Belgium

The present work evaluates hydrogen induced cracking in a TRIP-assisted steel with a complex multiphase microstructure, containing ferrite, bainite and retained austenite. When deformed, the retained austenite transforms to martensite and each structural constituent demonstrates a different behavior in the presence of hydrogen. The goal of this work is to understand the response of the hydrogen saturated multiphase structure to a mechanical load. Tensile tests on notched samples combined with in-situ electrochemical hydrogen charging were performed. The tests were interrupted at a stress just after reaching the tensile strength, since hydrogen induced cracks were found to form after reaching the tensile strength. Such interrupted tests allowed to study hydrogen induced crack initiation and propagation in the material. The microstructure of the samples was characterized by means of scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD). A correlation was found between the occurrence of martensite, which is known to be very susceptible to hydrogen embrittlement, and the initiation of hydrogen induced cracks. The latter were located on the surface in specific high-stressed regions, which were induced due to the presence of the notch.

MM 17.2 Mon 18:00 Poster E

Growth Process of Hydrogen Induced Structures on Gd Films and Islands Observed by STM — •Sara Wanjelik, Samuel Königshofen, and Mathias Getzlaff — Institute for Applied Physics, University of Düsseldorf

Hydrogen in metals as an area of research has been of great interest for the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamental point of view. But only few investigations are carried out by imaging techniques with a lateral resolution on the nm-scale. Even less works deal with the initial stage of hydride formation.

Here we present STM measurements on thin Gadolinium films and islands grown on a W(110) surface under ultra high vacuum conditions. On Gd-films two kind of hydrogen induced modifications can be observed: Hydrides and small disc-like islands with a diameter of a few nm and a height of one atomic step. The discs form chains with clearly preferred directions. A triangular shaped structure is observed together with the discs. The growth process of these modifications were studied in detail. Electronic differences of the described structures were investigated by maps of differential conductivity.

Contrary to films islands can be penetrated by hydrogen from the side walls. Therefore, the hydride formation should start from the edges. Another difference to films is that not only a vertical expansion, due to the larger volume of the hydride, is possible but also a lateral.

MM 17.3 Mon 18:00 Poster E

Kinetics of Hydrogen uptake in epitaxial thin films of Niobium — •Niklas Teichmann, Vladimir Burlaka, Stefan Wagner, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany.

Hydrogen located in interstitial lattice sites changes physical properties of the host metal, such as the resistivity or the lattice parameter.[1,2] Even though both physical properties are not linearly coupled to the hydrogen content, strong changes occur upon phase transitions. Therefore, they can be used to determine the concentration change and the onset of phase transition in thin films. In this paper we report on in-situ studies on the kinetics of the hydrogen uptake in thin Nb films (8 nm - 40 nm) with different Pd capping layers (0,2 nm - 20 nm). All experiments are performed without breaking the UHV conditions. Hydrogen is loaded step-wise from the gas-phase. It will be shown that even down to a Palladium capping layer thickness of 2 nm the kinetics of Hydrogen uptake is fast. It is dramatically reduced below that thickness. This effect is attributed to an island-like Pd-layer morphology that arises for the thinnest capping layer thicknesses. Also, the unloading kinetics is reduced when island-like capping layers are used.

Financial support by the DFG via projects PU131/9-1 and PU131/12-1 is gratefully acknowledged.

[1] A. Pundt, R. Kirchheim, Ann. Rev. Mater. Sci. 2006

[2] K. Nörthemann, & A. Pundt, (2008). Coherent-to-semi-coherent transition of precipitates in niobium-hydrogen thin films. Physical Review B, 78(1), 014105.

MM 17.4 Mon 18:00 Poster E

H-Diffusion in Mg-Fe11at% Alloys — •Magnus Hamm, Helmut Uchida, and Astrid Pundt — Universität Göttingen, IMP, Friedrich-Hund-Platz 1, 37077 Göttingen

In the last decade Magnesium (Mg) has attracted much interest as a storage material for hydrogen. The reasons are its high reversible hydrogen capacity of up to 7,6 wt% and its high volumetric capacity of 110 kg/m^3 [1]. However the slow hydrogen (de)absorbtion kinetics of Mg and its high desorption temperature provide a significant barrier to Magnesium's commercial use [2]. Iron (Fe) is known to improve the hydrogen uptake rate in Mg [3]. To study the influence of Fe on the kinetics of Mg, 500 nm Mg-Fe alloy films were prepared by Argon-ion-beam sputtering and loaded from the gas phase. The hydrogen uptake was studied in-situ with synchrotron radiation at DESY/Hamburg and ESRF/Grenoble. It will be demonstrated that the diffusion constant, while lower than in pure Magnesium, was orders of magnitude above the recorded diffusion constant of MgH2. In addition, with the used parameters full loading of the Mg-Fe samples is possible without any sign of a blocking layer. This differs strongly to what was found by H. Uchida et al.[4] on pure Mg films of similar thickness.

Beamtime provided at the DESY/Hamburg and the ESRF/Grenoble is gratefully acknowledged. This project is financially supported by the DFG via Project PU131/9-1 and PU131/10-1.

[1] Dornheim, R. et al., Scr. Mat. 56:10 (2007) [2] Bogdanović, B. et al., J. Alloys Compd. 282:1-2 (1999) [3] Holtz, R.L. and Imam, M.A., J. Mater. Sci. 34:11 (1999) [4] Uchida, H. et al., Acta Mat., accepted

MM 17.5 Mon 18:00 Poster E

Hydrogenography-Study of thin Vanadium-Hydrogen films — •Anshu Tyagi, Jantje Schommartz, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In this work, thin Vanadium films of 10 nm - 30 nm thickness, sputter deposited on transparent Glass substrates are examined. These samples are electrochemically loaded with hydrogen while simultaneous measurements of the transmission and reflection are done with a Light microscope. Electrochemical hydrogenography offers the possibility to study the local and the global hydrogen concentration within a defined area of the film and hence gives information on the lateral hydrogen distribution on a micrometer scale. Also the role of nucleation and growth in the hydrogenation of films is analyzed by using a mask technique during film deposition. In-situ Scanning Probe Microscopy studies are additionally performed. The role of the local detachment on the local hydride nucleation is examined by repeated loading experiments.

[1] J. Kürschner, S. Wagner, A. Pundt, Journal of Alloys and Compounds 593 (2014) 87-92. [2] L. Mooij, B. Dam, Phys. Chem. Chem. Phys. 15 (2012) 2782-2792. [3] J.L. Schommartz, Bachelor Thesis, University of Göttingen, (2014).

Financial support by the DFG via DFG-PU131/9-1 is gratefully acknowledged.

MM 17.6 Mon 18:00 Poster E

Optimized Pd/TiO_2 interfaces for high resolution TEM-EELS in H_2 atmosphere — •Marian Bongers, Carsten Nowak, and Astrid Pundt — Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

Redox reactions on supported metal catalysts exhibit high turnover rates [1, 2]. The used support strongly influences the turnover rate and, therefore, the metal/support interface is expected to be a very important parameter. Atomic resolution STEM and EELS allow to investigate the electronic states at Pd/TiO_2 interfaces, which are expected

to change under hydrogen atmosphere as suggested by Kobayashi et al. [3], thus eventually giving insight into the enhanced turnover rates.

Here we report on the preparation of optimized Pd/TiO_2 double layers. The layers were deposited by magnetron sputtering. XRD and texture measurements reveal epitaxial growth of a strained Pd-film on a single crystalline TiO_2 film.

EELS investigations on the electronic states in the vicinity of the Pd/TiO_2 interface are presented. Changes of the electronic states related to the presence of hydrogen are discussed. Additional EELS measurements on the oxygen edge show a strong dependency of the signal/noise ratio on the lamella thickness.

[1] D.C. Grenoble, M.M. Estadt, Journal of Catalysis 67 (1981) 90; [2] M. Bowker et al., Surface Science 497 (2002) 155; [3] H. Kobayashi et al., Surface Science 304 (1994) 393

Financial support by the DFG via SFB1073-C06 and DFG-PU131/9-1 is gratefully acknowledged.

MM 17.7 Mon 18:00 Poster E

Hydrogen-induced stress in ultrathin Nb-Fe Films — •Philipp Klose[1], Magnus Hamm[1], Helmut Klein[2], and Astrid Pundt[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Geowissenschaftliches Zentrum Göttingen, Goldschmidtstr. 1-3, 37077 Göttingen, Germany

Hydrogen which is located in interstitial lattice sites, is an origin for compressive mechanical stresses in thin films[1,2,3]. For low hydrogen concentrations, the in-plane film stress increases linearly on the hydrogen content.[3] Above a hydrogen-related yield stress the films deform plastically[4]. In this study, the hydrogen-induced stress development in niobium-iron (Nb_{90}-Fe_{10}) films is examined. The focus is on the thickness dependency of the stress development and the determination of the yield stress in these films.

The films of 3 nm - 40 nm were prepared by argon-cathode beam sputtering. They were studied by XRR-measurements to determine the exact film thickness. For selected samples the texture of the Nb-Fe films was determined by XRD to evaluate their epitaxial growth. Hydrogen loading was performed from the electrolyte using constant current conditions. The hydrogen concentration was determined via Faraday's law. The hydrogen-related yield stress is found to be strongly thickness dependent, in the thickness range studied.

[1] J. Weissmuller and C. Lemier, *Philos. Mag. Lett.* 80:6 (2000) [2] S. Wagner and A. Pundt, *Appl. Phys. Lett.* 92.5 (2008) [3] U. Laudahn et al., *JALCOM* 293-295 (1999) [4] A. Pundt, et al., *Phys. Rev. B* 61.15 (2000)

MM 17.8 Mon 18:00 Poster E

Correlation between thermodynamic and mechanical properties in binary bcc alloys — •Sandra Hoppe, Sascha B. Maisel, and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

When aiming at high-performance tailored metal alloys, it is crucial to understand basic material properties and their relation. Modern computer simulation methods like the cluster expansion with input from density functional theory calculations make the whole configurational space accessible. This way, also metastable structures may be considered, which are experimentally difficult to obtain. Recent results for several face-centered cubic (fcc) binary metal alloys [1] suggest a linear correlation between thermodynamic stability and elastic properties at a fixed stoichiometry. We investigated this relation between the formation enthalpy and the elastic constants c_{44} and c_{11} for several binary body-centered cubic (bcc) phases with alloying elements with bcc, fcc or hexagonal close-packed (hcp) equilibrium lattices and at different concentration regimes to understand the basic mechanisms behind this phenomenon. Interestingly, some alloys show similar trends to the fcc alloys, while Ta-W exhibits and anomalous behavior of c_{44} at the central concentration regime: Energetically favorable structures are mechanically less stable than those further away from the ground-state line.

[1] S. B. Maisel, M. Höfler, and S. Müller. *Nature* **491** (2012) 740.

MM 17.9 Mon 18:00 Poster E

A density functional theory study on elastic and thermodynamic characteristics of Al_5Fe_2 — •René Wirnata, Lilit Amirkhanyan, and Jens Kortus — Institute of Theoretical Physics, TU Freiberg, Deutschland

Based on density functional theory calculations, the η-Al-Fe binary phase of the quasi-crystal Al_5Fe_2 was studied. Since these calculations require an ideal crystal, an approximant for the starting structure [1], which contains channels of partially occupied sites, had to be constructed. Thermodynamic properties like the heat capacity at constant pressure and volume or the thermal expansion coefficient were calculated using the quasi-harmonic approximation. In addition, the elastic properties of this system as well as the magnetic Stoner criterion were analyzed.

For the heat capacity, the theoretical results could be compared with three experimental data sets [2,3,4]. In case the electronic contribution was incorporated, excellent agreement with two of these studies can be reported.

[1] U. Burkhardt et al., Acta Cryst. Sec. B **50**, 313-316 (1994)
[2] Ji Chi et al., Phys. Rev. B **82**, 174419 (2010)
[3] J. Seidel, TU Freiberg - Institute of Physical Chemistry
[4] T. Zienert, TU Freiberg - Institute of Material Sciences

MM 17.10 Mon 18:00 Poster E

On the atomistic diffusion processes in Cu65Zr35 metallic glass by molecular dynamics simulations — •Pablo Palomino[1], Giorgos Almyras[1], Dimitris Papageorgiou[2], and Giorgos Evangelakis[1] — [1]Department of Physics, University of Ioannina, Ioannina 45110 Greece — [2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece

Metallic Glasses (MG) are characterized by lack of long range order and periodicity. This particularity affects seriously most of their properties, including diffusion. Despite the serious research efforts in the last decades, both experimentally and theoretically, aiming in revealing the microscopic aspects of diffusion in MGs, several questions remain still open mainly referring to the diffusion mechanisms, the empty space required for a diffusion event to occur, the energetic requirements or the driving force, e.t.c.. In the present study we performed MD simulations on a well known model MG (Cu-Zr) focusing on the microscopic aspects of diffusion in both the supercooled and below the glass transition temperature regions. It came out that diffusion takes place by means of short distance atomic displacements, which become consecutive at high temperatures and are activated by the collective vibrations of neighboring atoms. Several relevant to diffusion processes quantities were evaluated, quantified and compared with available data in the literature in the whole temperature region studied. We think that the present results could be used to enlighten phenomena related to slow diffusion like aging or creep relaxation.

MM 17.11 Mon 18:00 Poster E

In-situ Delithiation of $LiMn_2O_4$ by Laser Assisted Atom Probe Tomography — •Jonas Arlt, Björn Pfeiffer, Johannes Maier, and Carsten Nowak — Georg-August-Universität Göttingen, Institut für Materialphysik, 37077 Göttingen, Germany

Manganese dioxides have been extensively studied as cathodematerial in rechargeable Li-ion batteries. Understanding ionic conduction and energy conversion processes in the cathodematerial is crucial for the optimization of Li-ion batteries. Current experimental data is usually obtained with methods characterizing transport on a macroscopic scale, but particularly for phase separating materials transport is expected to be strongly localized. To overcome this, atom probe tomography (APT) and related techniques have been further developed to obtain local information on the chemical composition and ionic transport with sub nm resolution [1, 2].

Here, we present Laser-APT studies on $LiMn_2O_4$. Modifying the experimental conditions during the measurement allows in-situ studies of the delithiation process, revealing insights into ionic transport mechanisms. Using a focused ion beam, nanoscopic $LiMn_2O_4$ tips were prepared. Sample morphology and crystal structure were determined by transmission electron microscopy. The influence of the applied electric field, temperature and laser parameters on the delithiation process will be discussed.

References

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[2] C. Escher et al., *Phys. Rev. Lett.* **97**, 136601 (2006).

MM 17.12 Mon 18:00 Poster E

Probing magnetic phase transitions in Heusler-alloys and Magnetite using EMCD — •Walid Hetaba[1,2], Stefan Löffler[1], Michael Stöger-Pollach[1], Andreas Hütten[3], Gareth Parkinson[4], Marc-Georg Willinger[2], and Robert Schlögl[2] — [1]USTEM, Vienna University of Technology, Austria — [2]Department of Inorganic Chemistry, Fritz Haber Institute of the MPG, Berlin, Germany — [3]Thin Films and Physics of Nanostructures, Department of Physics, Bielefeld University, Germany — [4]Institute of

Applied Physics, Vienna University of Technology, Austria

Energy-loss magnetic chiral dichroism (EMCD) is a versatile technique to investigate magnetic properties on the nanoscale. Heusler-alloys and Magnetite are promising systems in the field of spintronics. Furthermore, multilayer Heusler systems are used for ferroic cooling applications. These alloys show an austenitic-martensitic phase transition, where the transition temperature depends on the actual elemental composition. Magnetite shows a Verwey transition at about 120 K. In this work, we perform in-situ EMCD measurements to investigate the changes of the magnetic properties at different temperatures. The experimental results are found to be in very good agreement with simulations. These simulations are crucial as dynamical diffraction affects the intensity of the measured EMCD signal, bringing the sample thickness into the game. By combining theory and experiments, this study paves the way for tailoring the magnetic phase transition of materials for the use in spintronics. The Austrian Science Fund is acknowledged for financial support under grant numbers F4501-N16 and I543-N20.

MM 17.13 Mon 18:00 Poster E

Resolution analysis of Transmission Kikuchi Diffraction (TKD) patterns in SEM — •Dennis Langenkämper, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Since the first commercial systems appeared in the early 1990s, electron back-scatter diffraction (EBSD) has grown into one of the most common techniques to characterize the microstructure of crystalline samples. Due to its ease and vast range of applicability to materials in the submicrometer grain size range, EBSD is a widely spread method to analyze deformation structures and mixtures of phases.

Current research focuses on nanoscaled materials, which may show drastic changes in properties with often superior results. Thus, there is a strong need to enhance the spatial resolution of EBSD. Transmission Kikuchi Diffraction (TKD) is a suitable method to overcome limits of EBSD by using thin samples transparent to the electron beam.

The present work focuses on the resolution limits, using a conventional EBSD detector (EDAX) and a custom-build TKD sample holder to study the influence of experimental conditions (sample thickness, sample material) on the resolution limit of TKD.

MM 17.14 Mon 18:00 Poster E

Non-isothermal crystallization kinetics of metallic glass by differential fast scanning calorimetry — •Bin Yang[1], Yulai Gao[2], and Christoph Schick[1] — [1]AG Polymer Physics, Institute of Physics, University of Rostock, Germany — [2]School of Materials Science and Engineering, Shanghai University, Shanghai, P.R. China

The thermal stability and the kinetic fragility of Al86Ni6Y4.5Co2La1.5 (%wt.) metallic glass were investigated by ultra-fast non-isothermal thermal analysis. The differential fast scanning calorimeter (DFSC) traces revealed that the material undergoes a three-stage crystallization for heating rates ranged from 5 to 40,000 K/s. Combining DSC and DFSC, the kinetics of the glass transition and crystallization of Al86Ni6Y4.5Co2La1.5 metallic glass was investigated. The kissinger plot can express the temperature dependence of growth rate of this metallic glass. Furthermore, the kinetic fragility for Al86Ni6Y4.5Co2La1.5 metallic glasses is evaluated. Depending on the fragility index, this metallic glass is a liquid of very high fragility, similar to several organics.

MM 17.15 Mon 18:00 Poster E

Low frequency acoustic measurements on the metallic glass $Zr_{46.8}Ti_{8.2}Cu_{7.5}Ni_{10}Be_{27.5}$ — Sebastian Craft, •Arnold Seiler, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

The properties of amorphous solids at low temperatures are well known to be dominated by atomic two-level tunneling systems (TS). While the standard tunneling model successfully describes thermodynamic properties of insulating glasses it fails to predict the elastic properties of metallic glasses. To investigate the role of conduction electrons on the density of states and the dynamics of TS vibrating reed experiments are performed. In superconducting glasses the interaction can be switched on and off by means of a magnetic field which suppresses superconductivity and therefore enables electrons to interact with TS. Here we present measurements of the internal friction and the sound velocity of the splat cooled superconducting metallic glass $Zr_{46.8}Ti_{8.2}Cu_{7.5}Ni_{10}Be_{27.5}$ measured at frequencies between 600 Hz and 14 kHz and temperatures from 10 mK to room temperature. Within these experiments we used an improved sample geometry to reduce clamping losses and to excite different modes at various frequencies.

MM 17.16 Mon 18:00 Poster E

Impact of minor-alloying on the mechanical properties of Pd-based bulk metallic glasses — •Niklas Olschewski, Niklas Nollmann, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Metallic glasses offer unique properties such as high strength, extended elasticity, high wear and corrosion resistance. However, the limited ductility and especially the immediate catastrophic failure in tension once the elastic limit is reached are major obstacles to applications as structural materials. This behavior has led to substantial effort towards understanding and improving the accommodation of plastic deformation in metallic glasses, including the design of composites consisting of glassy material surrounded by ductile crystallites. Our work has focused on the improvement of the ductility of bulk metallic glasses by adding minor alloying elements. In particular the impact of adding slight amounts of cobalt or iron (0.2 - 4 wt.%) to the well-known bulk glass-former $Pd_{40}Ni_{40}P_{20}$ on the mechanical properties has been studied.

The samples were produced by copper mold casting and their mechanical behavior was tested in compression and three-point bending tests. Further investigations (e.g. DSC, XRD, ultrasonic measurements, SEM) have been conducted to characterize the alloys' properties. The obtained results are discussed.

MM 17.17 Mon 18:00 Poster E

Processing and characterization of a deformed ZrCu metallic glass with tunable content of nanocrystallites — •Marius Gerlitz, Jonas Bünz, Martin Peterlechner, and Gerhard Wilde — Westfälische Wilhelms-Universität, Münster, Deutschland

The deformation mechanisms of metallic glasses are in focus of current research. In the present work, a ZrCu-based glass with a nominal composition of $Zr_{53.8}Cu_{31.6}Ag_{7.0}Al_{7.6}$ (at. %) was processed by arc melting and subsequent melt-spinning. Upon heating, controlled growth of crystallites occurs at well-chosen temperatures and times. A study is carried out by systematically varying the annealing parameters of the as-produced amorphous sample using differential scanning calorimetry (DSC). Determination of the crystallization kinetics leads to the ability to tailor the volume fraction of nanocrystallites embedded in the amorphous matrix. The obtained nanocrystallites are observed by transmission electron microscopy (TEM). Subsequently to an annealing treatment to obtain partial crystallization, the material is deformed by cold rolling using a two-high rolling mill. This method leads to the generation of shear bands. TEM analysis was carried out to analyze shear bands and their interaction with nanocrystallites. The results are discussed with respect of the impact of nanocrystalline precipitates on the propagation of shear bands in a metallic glass.

MM 17.18 Mon 18:00 Poster E

Liquid Metallic Hydrogen and Solar Physics — •Alexander Unzicker — Pestalozzi-Gymnasium München

The metallic state of hydrogen, postulated by Wigner and Huntigton in 1935, presents both experimental and theoretical challenges and is a topical research field in condensed matter physics. In particluar, it has been hypothesized that liquid metallic hydrogen may be metastable at normal conditions. Focussing on the unique character of hydrogen as 'zeroth' alkali metal, the ranges of possible pressures and temperatures are discussed.

The existence of a metastable state would have profound consequences for understanding of the sun, since a series of observations supports the idea that the sun's surface is liquid. These arguments have been advanced in much detail by Pierre-Marie Robitaille, a renowned radiologist, but have received little attention in the solar physics commmunity so far.

The talk also tries to enhance the communication across different fields of physics that is sometimes necessary when a long established paradigm - in this case the standard solar model - is in trouble. Disussions are particlularly welcome.

MM 17.19 Mon 18:00 Poster E

Thermally induced hydrogen desorption of metal-borohydrides — Christoph J. Sahle[1], Simon Kujawski[2], Arndt Remhof[3], Yigang Yan[3], Nick Stadie[3], Kolja Mende[2], Ali Al-Zein[1], Simo Huotari[4], Metin Tolan[2], and •Christian Sternemann[2] — [1]European Synchrotron Radiation Facility, Greno-

ble, France — [2]Fakultät Physik / DELTA, Technische Universität Dortmund, Dortmund, Germany — [3]Empa, Hydrogen and Energy, Dübendorf, Switzerland — [4]Department of Physics, University of Helsinki, Helsinki, Finland

Complex lightweight hydrides are candidates for efficient reversible hydrogen storage. During dehydrogenation the hydrides decompose into both crystalline and amorphous phases where latter are often difficult to detect. We use x-ray Raman scattering, a bulk sensitive probe of soft x-ray absorption edges, to measure e.g. boron K- and magnesium L-edges both ex-situ and in-situ during decomposition. To clarify possible decomposition pathways, spectra of reference samples are employed to fingerprint intermediate phases via principal component analysis. Results for magnesium and calcium borohydrides will be discussed with focus on the formation of closo-borane species, which could act as a boron sink and hinder cycling.

MM 17.20 Mon 18:00 Poster E

Potential-strain coupling during hydrogen electroabsorption — •Shan Shi[1], Tobias Kitzler[1], Qibo Deng[2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Insitut für Werkstoffforschung, Werkstoffmechanik — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

The recent past has seen an increasing interest in the impact of mechanical deformation on the electrode processes. The effect is measured by the potential-strain coupling coefficient (ς) which quantifies the variation of the electrode potential, with tangential strain. In this study, we use dynamic electro-chemo-mechanical analysis (DECMA) to determine the potential-strain coupling during hydrogen electroabsorption into a Palladium (Pd) thin film. The samples are prepared by DC magnetron sputtering of a nanometer thick Pd film, which contains many grain boundaries, on a polyimide substrate. We monitor the electrochemical behaviour of the Pd thin film in aqueous electrolytes during imposing periodical elastic strain on the sample. Additionally, another customised in-situ electrochemical cell enables us to determine microstructural information of the Pd film such as the lattice parameter by in-situ X-ray diffraction. By combining the results, the question how the mechanical strain affects the storage of light interstitials (H) in Pd and the kinetics of the adsorption or dissolution at the electrode surface and the absorption in the grain boundaries and the bulk will be explored.

MM 17.21 Mon 18:00 Poster E

In-situ TEM of phase transitions in TiNi based shape memory alloys — •Timo Wuttke and Cynthia Ann Volkert — Institute of Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Shape memory alloys (SMA) are known for their ability to recover plastic deformation upon heating and thus may be used for applications such as actuation in a wide range of industry, science and medical related fields.

The key mechanism responsible for this behavior is a reversible diffusionless solid-state phase transition between a highly twinned martensitic state and an untwinned austenitic phase of higher crystal symmetry.

We studied the martensitic phase transition of TiNi and TiNiCu alloys utilizing in-situ TEM techniques. Both commercially available wires and samples prepared with vacuum arc melting were used. All samples were annealed at 600°C for 1,5h and water quenched to ensure that the phase transition takes place between RT and 100°C thus making it easily accessible in the TEM.

The movement of the austenite-martensite reaction front can be directly observed and manipulated by applying temperature gradients to the TEM lamella. This allows us to study the phase transformation with high spatial resolution. Atomic level information obtained at the moving phase boundary using HRTEM will be discussed.

MM 17.22 Mon 18:00 Poster E

Gas sensors based on metal oxides deposited on AAO for the detection of carbon monoxide — •Jonas Lübke, Stefan Ostendorp, Nina Winkler, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

Carbon monoxide is a colourless, odourless, flavourless and non-irritant gas produced from partial oxidation of carbon-containing compounds. If inhaled, it connects to the central iron atom of haemoglobin and therefore prohibits oxygen transport in blood, which leads to death by choking. Therefore sensitive and reliable detection is of great interest. Carbon monoxide acts reductive on most oxidized semi-conductors (SC's), leading to increased or decreased resistance, depending on whether they are n- or p-type SC's. Former work has shown successful detection of CO with metal oxide semi-conductors (MO-SC) on glass substrates. To increase the detecting surface and the inspected volume, use of "Anodic Aluminum Oxide" (AAO)-membranes as substrate seems to be promising. To this end, metal oxides were deposited on AAO via atomic layer deposition (ALD). The gas sensor set-up is brought into a temperature-controlled vacuum chamber to provide the required activation energy for chemisorption of CO in a defined gas environment. A well-defined amount of air is introduced to the chamber and then a well-defined amount of CO. The current through the sample/gas sensor is measured via a four probe measurement. The effect of modifications of the membranes and oxide films concerning the resultant gas sensing properties was examined.

MM 17.23 Mon 18:00 Poster E

A novel kind of solid state thin film battery — •Yaser Hamedi Jouybari and Frank Berkemeier — Institute of Material Physics, Westfälische Wilhelms-Universität Münster, Münster, Germany

Thin film lithium batteries (TFBs) are regarded as next Generation of energy storage devices for highly specialized applications. In our work we investigate a novel kind of TFB that consists of high-performance active materials. In particular, we are using thin films of LiFePO4 as cathode, LiPON as solid electrolyte, and silicon as anode. All materials are prepared by sputtering, to achieve a well-defined thickness and uniformity of the layers. To investigate the electrochemical behavior of these TFBs, the overall battery cells, as well as the individual battery components, are studied by transmission electron microscopy, atomic force microscopy, cyclic voltammetry, chronopotentiometry, and impedance spectroscopy.

In our studies it turned out that the transport across the interfaces between the electrolyte and the electrodes is most critical to TFB performance. This transport is heavily affected by some disturbing phenomena such as unwanted reaction layers, roughness of the solid electrolyte, and its degradation during subsequent deposition processes. To increase the interface quality, all of these phenomena need to be minimized and controlled by deposition parameters. Hence, in our work we report on the dependence of the TFBs performance on the deposition parameters, with particular focus on the properties of the LiPON under different deposition conditions.

MM 17.24 Mon 18:00 Poster E

Atomistic simulations of materials relevant for nuclear waste management — •Yaqi Ji, George Beridze, Yan Li, and Piotr Kowalski — Institute of Energy and Climate Research: IEK-6 Nuclear Waste Management and Reactor Safety, Forschungszentrum Jülich, Jülich, Germany

Safe management of nuclear waste represents a challenge for nuclear energy utilizing countries. Thus, a significant research effort has been devoted to investigate the potential solid nuclear waste forms in which radionuclides could be immobilized under repository conditions and stored for even geological times. The goal of such research is the full characterization of properties of these materials upon incorporation of actinides into their crystalline structures. One challenge related to the atomistic modelling of these strongly correlated materials is the proper description of their electronic structure. In that aspect we present our results on benchmarking the DFT+U method for derivation of the thermochemical properties of actinide-bearing molecular compounds and solids [1] and its application to the computer-aided characterization of the potential disposal waste form materials such as monazite-type ceramics ($Ln\mathrm{PO}_4$) and pyrochlore [2,3]. In particular we will present results of investigation of the thermodynamic stability of these ceramics [3] under potential repository conditions and simulations of radiation damage effects in these materials.

[1] Beridze. G. & Kowalski, P. M., J. Phys. Chem. A. in press (DOI: 10.1021/jp5101126) [2] Blanca-Romero, A. et al, J. Comput. Chem. 35, 1339 (2014). [3] Li, Y. et al., J. Solid State Chem. 220,137 (2014).

MM 17.25 Mon 18:00 Poster E

3D nanofabrication of subsurface structures inside photosensitive glass with fs laser — •Tobias Milde[1], Ulrike Brokmann[2], Edda Rädlein[2], and Klaus Liefeith[1] — [1]Department of Biomaterials, Institute for Bioprocessing and Analytical Measurement Techniques Heiligenstadt — [2]Group of Inorganic-Nonmetallic Materials, Department of Mechanical Engineering, Technische Universität Ilme-

nau

The development of miniaturized structures on or below the surface of glass is an issue of present research. Femtosecond-laser-radiation combined with the two photon process is a promising approach to push the written structures towards the nanometer scale. Here we used the photosensitive glass FS21 with its three step photoform process (irradiation, annealing, HF-etching). For the irradiation we used a TiSa oscillator only. These structures and steps are developed to realize a distinct miniaturization of glass components and to improve biocompatibility for specific cells. This structured glass is interesting for microfluidic and lab-on-a-chip devices. Here we present new scientific findings to material characterization and the photoform process.

MM 17.26 Mon 18:00 Poster E

Phase equilibria and interfacial properties of a curved liquid-solid interface — •Muhammad Ajmal Choudhary[1], Julia Kundin[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth — [2]Institut für Angewandte Physik, Universität Tübingen, D-72076 Tübingen

The phase field crystal (PFC) technique is a novel approach for modeling crystal growth phenomena with atomistic resolution on mesoscopic time scales. We use a 2D PFC model for a binary system based on Elder et al. [Phy. Rev. B 75, 064107 (2007)] to establish a precise assessment of the nucleation mechanisms beyond classical nucleation theory. More specifically, we investigate the equilibrium properties of a curved liquid-solid interface as well as the nucleation barriers. We propose the method of determining interfacial energies for a curved liquid-solid interface in a finite system by stabilizing the circular solid crystal of various radii in the surrounding liquid phase and liquid droplets of various radii in the corresponding solid phase. We suggest a phenomenological expression to describe the dependence of the extracted interface tension on the nucleus radius r for the liquid-solid system. The numerical PFC results show that this dependency can not be fully described by the non-classical Tolman formula. Moreover, we also derived the free energy barriers for the nucleation and compared the results with predictions based on classical nucleation theory.

MM 17.27 Mon 18:00 Poster E

Atom probe tomography studies of the effects of industrial heat treatment on the precipitation kinetics on aluminum alloy 2195 — •Muna Khushaim[1], Judith Seibert[2], Ferdinand Haider[2], and Talaat Al-Kassab[3] — [1]Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia. — [2]University Augsburg, Inst. f. Physics, D -86159 Augsburg, Germany. — [3]D-37077, Göttingen, Germany.

Aluminum lithium alloys are of great interest for commercial, military and aerospace applications. These alloys possess high strength, light weight, low density and good mechanical properties.The superior mechanical properties of this alloy is owing to the presence of different intermetallic phases such as T_1 (Al_2CuLi), $\theta^{'}$ (Al_2Cu), $\delta^{'}$ (Al_3Li) and $\beta^{'}$ (Al_3Zr).The objective of this work is to provide insight into the relationship between precipitation sequences, mechanical properties and the preformed heat treatment conditions. Aluminum alloy 2195 was selected as a model system in the present study. Different industrial heat treatments such as: T8 temper, T4 temper and T6 temper were applied on the alloy. Utilizing laser assisted wide angle tomographic atom probe (LAWATAP) and local electrode atom probe (LEAP) allowed the investigation of precipitation kinetics and phase transformation phenomena. Data will be presented will highlighting the role of the industrial heat treatment on the developing of the microstructure, along with an in depth study of distribution of different alloying elements in the strengthening phases.

MM 17.28 Mon 18:00 Poster E

Microstructure and electrical characterization of commercial Na-β-Alumina — •Wolfram Münchgesang[1], Torsten Schucknecht[2], Barbara Abendroth[1], Tilmann Leisegang[1,3], David Rafaja[2], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Freiberg, Germany — [2]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Freiberg, Germany — [3]Fraunhofer-Technologiezentrum Halbleitermaterialien THM, Freiberg, Germany

Na-β-Alumina (NaBA) is a well-known and commercially available solid electrolyte (SE) for high-temperature Na-S-accumulators (NSA). Under conditions of standard working temperatures of around 300 °C NaBA is stable, electrically insulating and ion-conducting.

These properties make NaBA also interesting for low-temperature NSA, as an alternative separator and as a reference for SE. The challenge for the transfer from a high- to a low-temperature working SE is to compensate the strong decreased ion-conductance by a decreased thickness, without reducing its stability and insulating properties. In this regard, the microstructure of NaBA and its influence on the conductivity has to be worked out and controlled during preparation.

We will present and discus results on multiscale investigation of commercial NaBA exhibiting a complex defect structure. This involves the analysis of the chemical and phase distribution as well as the microstructure and their influence on the conductivity.

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MM 17.29 Mon 18:00 Poster E

Pressure-induced spin transition of Fe^{2+} in siderite $FeCO_3$ studied by x-ray Raman scattering — •Christopher Weis[1], Christian Sternemann[1], Max Wilke[2], Valerio Cerantola[3], Christoph J. Sahle[4], Georg Spiekermann[5], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Helmholtz-Zentrum Potsdam, German Research Centre for Geoscience (GFZ), 14473 — [3]Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany — [4]ESRF, 38043 Grenoble Cedex 9, France — [5]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Pressure-induced electronic and/or structural transitions of iron bearing compounds at conditions of the inner earth fundamentally affect the material's properties, e.g. sound velocitiy and density. Siderite ($FeCO_3$) forms a complete solid solution with magnesite ($MgCO_3$). Owing to the low solubility of carbon in the mantle it is a candidate for carbon storage and a key mineral to understand the Earth's carbon cycle. Lavina et al. [1] applied high-pressure x-ray diffraction to siderite and found a high-spin to low-spin transition to occur at 43-49 GPa with a sharp volume collapse of 10 % at a pressure of 44 to 45 GPa. We investigated changes in the electronic structure of a siderite single crystal for pressures up to 50 GPa using a Boehler-Almax diamond anvil cell with helium as pressure medium by x-ray Raman scattering at the iron $M_{2,3}$-edge and $L_{2,3}$-edge. The course of the spin transition up to 50 GPa is discussed by the observed spectral changes. [1] B. Lavina et al., Geophys. Res. Lett. 36, L23306 (2009)

MM 17.30 Mon 18:00 Poster E

Real space morphological analysis of multilevel domain structures in polycrystalline ferroelectric relaxors — •danka gobeljic[1], vladimir v shvartsman[1], sergei v kalinin[2], stephen jesse[2], and doru c lupascu[1] — [1]Institute for Material Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Essen, Germany — [2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA

The local domain configuration and its dynamics play a vital role in the properties of ferroelectric materials. Therefore, domain architectures have been subject to systematic theoretical and experimental studies. The expected regularity of domain patterns is often distorted in real materials. In particular, this is typical for system with inherent disorder, e.g. for relaxors. Maze-like domain structures have been reported for the latter. To extract quantitative characteristics of such complex domain patterns one needs a special analytical tool. We introduce the quantitative line-of-sight (LoS) domain structure analysis. Based on 2D spatial maps of domain structures obtained by piezoresponse force microscopy (PFM), the LoS provides a quantitative measure of the characteristic domain shape, size, and spatial organization. We demonstrate the validity of this technique for Bi1/2Na1/2TiO3-BaTiO3 based relaxor ceramics. The parameters of the complex domain morphology are discussed in the context of grain orientation and local composition.Beyond comprehensive investigation of the local properties, LoS is applied as a comparative tool in the study of the macroscopic properties of the investigated ceramics.

MM 17.31 Mon 18:00 Poster E

Molecular dynamics simulation of the α-γ phase transition in iron-nickel system — •Emilia Sak-Saracino and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS,Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Germany

Using molecular dynamics simulation, we study the austenite-martensite phase transition in the iron-nickel system. During a heat-

ing/cooling cycle, the phase transition can be observed by monitoring the hysteresis of the system volume with temperature. We find that with increasing nickel concentration, the martensite and austenite temperatures decrease, in agreement with experiment.

MM 17.32 Mon 18:00 Poster E

Theoretical modelling of the electronic structure of MAX phases using WIEN2k and calculation of electric field gradients — Daniel Jürgens[1], Michael Uhrmacher[1], Jose Mestnik-Filho[2], and •Hans Hofsäss[1] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, Sao Paulo, Brazil

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds. In this work, we us the program WIEN2k to calculate electric field gradients (EFG) for In or Hf probe atoms on either A-or M-sites in different MAX phases. We present comprehensive calculations of EFGs in many 211-MAX phase compounds and compare with our experimental results from perturbed angular correlation measurements. We discuss the dependence of the A-site EFGs as function of the A-Element ranging from Al to Pb and for M-elements ranging from Ti to Hf. We find a characteristic dependence of the EFG strength on the M-element valence electron density. In most of the investigated MAX-phases we can quantitatively predict the EFG for probe atoms on A- or M-sites with good accuracy. This makes perturbed angular correlation an ideal and universal method to study electronic and also possible magnetic properties of MAX phases.

MM 17.33 Mon 18:00 Poster E

Investigations of electric field gradients at A-sites in the 312- and 413-MAX-phases using perturbed angular correlation spectroscopy — Daniel Jürgens[1], Michael Uhrmacher[1], •Hans Hofsäss[1], and Michael W. Barsoum[2] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Department of Material Science and Engineering, Drexel University, PA, USA

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds, which are known for their metallic as well as their ceramic properties. The perturbed angular correlation (PAC) was used to determine the local environment of implanted probe atoms on atomic scale. The compounds Ti_3AlC_2, Ti_3SiC_2, Ti_4AlN_3 and Ta_4AlC_3 were investigated with PAC using implanted 111In probe atoms., which occupy A-sites after annealing the implantation damage. In this study we investigate dependence of the strength of the electric field gradient (EFG) on the stacking sequence of the laminar MAX phases. The comparison of EFGs measured in the different sub-groups of MAX phases show that the EFGs in the 413 phases are slightly smaller compared to the corresponding 211 phase. Increasing the M-X intermediate layer thickness while going from M_2X to M_3X_2 to M_4X_3 phases reduces the EFG strength at the A-Site. This behavior allows a characterization of stacking sequence variations occurring e.g. in thin film MAX phases.

MM 17.34 Mon 18:00 Poster E

Electric field gradients at M- and A-sites in 211 MAX-phases using perturbed angular correlation spectroscopy — Daniel Jürgens[1], Michael Uhmacher[1], Ulrich Vetter[1], Matthias Nagl[1], •Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michael W. Brasoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, Sao Paulo, Brazil — [3]Department of Material Science and Engineering, Drexel University, PA, USA

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds, which are known for their metallic as well as their ceramic properties. Since most techniques only allow a macroscopic insight, the perturbed angular correlation (PAC) was used to determine the local environment of implanted probe atoms on atomic scale. Radioactive ^{111}In and ^{181}Hf ions, both decaying by a $\gamma-\gamma$ cascade, were implanted into Zr_2InC and Hf_2InC and the electric field gradients (EFG) at a A-site (in) and M-sites (Hf) were measured after annealing the implantation damage. We report on the different annealing behavior observed for In and Hf probes. We compare the results with density functional theory calculations and give reasons for dissimilar EFGs at A- and M-sites. Further results for other 211 MAX-phases (Ti_2InC, Ti_2AlC, V_2AlC, Cr_2AlC, Nb_2AlC, Ti_2AlN,Cr_2GeC, Ti_2GeC,Nb_2AsC, and Ti_2SiC) are presented.