MM 26: Poster session II

Posters should be displayed by 4 pm. The MM poster price will be awarded during the annual general assembly on Wednesday evening.

Posters submitted to: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science, Electron Microscopy of Materials, Interfaces, Functional Materials, Nanomaterials, Caloric Effects in ferroic materials

Time: Tuesday 18:30–20:30 Location: Poster B3

MM 26.1 Tue 18:30 Poster B3

Mechanical behavior of fivefold twinned silver nanowires by means of *in situ* tensile tests in the TEM — •Nadine Schrenker[1], Mirza Mackovic[1], Manuela Göbelt[2], Silke Christiansen[2,3], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany — [3]Helmholtz Centre Berlin for Materials and Energy, Germany

Organic (opto)electronics have recently undergone a rapid development. Major advantages compared to their inorganic counterparts are that they can be manufactured on flexible substrates. Silver nanowire (Ag NW) films are highly promising as flexible transparent electrodes, e.g., for organic solar cells, as they fulfill the requirement of a low sheet resistance combined with a high transparency. Indium tin oxide (ITO), which is still the most common used material, behaves brittle under deformation and is relatively expensive. On a macroscopic scale bending tests revealed the excellent performance of Ag NW films, since the increase of resistance is small compared to ITO films. To complement the macroscopic bending tests, understand failure mechanisms and prospectively optimize the deformation behavior of AgNW electrodes *in situ* mechanical testing in the TEM are conducted. On a nm scale tensile tests of single 5-fold twinned Ag NWs show a ductile behavior and a size effect of the strength. Moreover, microscopic *in situ* tensile tests of individual junctions and areas on the μm scale of AgNW films in the TEM are in focus of our current research.

MM 26.2 Tue 18:30 Poster B3

Surface Nucleation Controlled Plasticity in Twinned Gold Nanowires — •Zhuocheng Xie, Jakob Renner, Aruna Prakash, and Erik Bitzek — Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Science & Engineering, Institute I, Erlangen, Germany

Metallic nanowires (NWs) receive currently much attention due to their often superior mechanical properties compared to bulk materials. Similarly, nanotwinned metals have lately attracted a lot of interest because they combine high strength with high ductility, two properties which have been thought to be mutually exclusive. Recently, nanotwinned nanowires were reported, which could combine both strengthening mechanisms, namely surface dislocation nucleation controlled plasticity and hardening due to dislocation - twin interactions.

Here, we report on molecular dynamics simulations of tensile tests on single and multi-twinned Au nanowires with <110> and <112> orientations. The interactions of partial dislocations nucleated at the surfaces with the twin boundaries parallel to the wire axis are analyzed in detail and the resulting deformation behavior is compared to recent experiments.

MM 26.3 Tue 18:30 Poster B3

Investigation of perovskite interfaces with negative spherical aberration in HRTEM — •Tobias Meyer[1], Patrick Peretzki[1], Benedikt Ifland[2], Christian Jooss[2], and Michael Seibt[1] — [1]IV. Physical Institute, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Materials Science, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The well-known Shockley-Queisser limit for the efficiency of single junction solar cells is based on energy losses due to transmission of low energy photons and thermalization of highly excited charge carriers. To overcome these limitations semi-conductors with small band gaps and long relaxation times are desirable. Long living states of small polarons have been observed in strongly correlated perovskite materials of the general form $A_{1-x}A'_xBO_3$. The properties of these systems are related to orbital, charge and magnetic ordering phenomena which are highly dependent on the doping level and the particular choice of A, A', and B. In the perfect perovskite lattice the B-site ion is centered in an octahedral spanned by the surrounding oxygen anions. Cooperative distortions and tilts of the octahedral affect the ordering phenomena and can also lead to relaxations of e.g. epitaxial strain. Junctions between $Pr_{0.67}Ca_{0.33}MnO_3$ (PCMO) and $SrTiO_3$ (STO) have been investigated in an image corrected TEM using negative spherical aberration imaging (NCSI) combined with focal series recording. Object waves reconstructed from such focal series were processed to study oxygen vacancies as well as octahedral tilts and distortions induced by the slightly different lattice parameters of PCMO and STO.

MM 26.4 Tue 18:30 Poster B3

Exploring the friction between atomic layers with *in situ* SEM mechanical testing — •Peter Schweizer, Florian Niekiel, and Erdmann Spiecker — Center for Nanoanalysis and Electron Microscopy (CENEM), University of Erlangen-Nuremberg, Cauerstr. 6, 91058, Erlangen, Germany

With the advent of nano-electromechanical systems, the understanding of atomic-scale friction becomes very important, since the life-time and functionality of such systems is often limited by the effects of friction and wear. Interfaces made of flat atomic layers can in certain conditions show the effect of ultra-low friction, also referred to by the term of "superlubricity", which might alleviate the tribological problems that NEMS face today. However there are still a lot of open questions regarding friction on the atomic scale, especially the evolution of the microstructure in an interface during sliding.

In this work we present an approach to quantitatively measure the friction forces between atomic layers, using vanadium diselenide (VSe_2) as a model system. Following a preparation routine with the focused ion beam area dependent friction forces are measured *in situ* in the scanning electron microscope with the help of a micro-manipulator and a spring table. The microstructure of the interface is analyzed after sliding using transmission electron microscopy. Different crystallographic orientations of the tribological interface are compared and links to the microstructure are drawn.

MM 26.5 Tue 18:30 Poster B3

Self-assembly of an imidazole-based ligand on Au(111) and on Cu(111) — •Patrick Seitz[1], Nico Fritsch[2], Thomas Waidmann[2], Nicolai Burzlaff[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany

Imidazole-based ligands are versatile building blocks to form one-dimensional coordination polymers on surfaces [1,2]. In this work, the self-assembly and conformation of 1,2-bis(*N*-methylimidazol-2-yl)ethylene ligands on Au(111) and Cu(111) was studied using low temperature scanning probe microscopy (STM) in ultra-high vacuum. The subtle balance between intermolecular and molecule-surface interactions determines, whether the molecules adsorb as *cis*- or *trans*-isomers. On Au(111), the molecules interact with one another through hydrogen bonds. We observe dimers and trimers formed from *cis*-isomers while *trans*-isomers self-assemble in one-dimensional chains at submonolayer and two-dimensional islands at monolayer coverage. In contrast, the molecules preferably adsorb as monomers on Cu(111) owing to a strong molecule-surface interaction. [1] Fischer et al., Chemistry - A European Journal, 2011, 17 (34), 9293-9297 [2] Fritsch et al., Inorganic Chemistry, 2014, 53 (23), 12305.

MM 26.6 Tue 18:30 Poster B3

Deformation behavior and solid solution strengthening of metallic micro- and nanoparticles studied by in situ electron microscopy — •Patrick Herre[1], Stefan Romeis[1], Jonas Paul[1], Mirza Mačković[2], Florian Niekiel[2], Simon M. Kraschewski[2], Erdmann Spiecker[2], and Wolfgang Peukert[1] — [1]Institute of Particle Technology (LFG), Friedrich-Alexander-Universität Erlangen-

Nürnberg, 91058 Erlangen, Germany — [2]Institute of Micro- and Nanostructure Research (IMN), Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The small scale deformation behavior of (sub-) micron particles and structures is fairly distinct from the bulk due to internal and external interfaces as the size dimensions are close to the characteristic length scale (e.g. dislocation spacing) of the underlying physical (deformation) mechanism. In order to deepen the current understanding of small scale mechanics, metallic particles of defined size, morphology, structure and composition are synthesized by liquid and solid state dewetting of thin metallic films on ceramic substrates. As a model and reference system, thin Au films are dewetted on (0001) sapphire substrates. Hence, single-crystalline and defect-free Au particles of defined shape and orientation with respect to the substrate are obtained and depict an ideal specimen for decent mechanical testing. In addition, thin films composed of pure Ni as well as Ni-rich solid solutions of Ni-Ta and Ni-W are prepared via electron beam PVD on sapphire substrates. In situ electron microscopy is used as a powerful tool for conducting deformation experiments of adequate image and data resolution.

MM 26.7 Tue 18:30 Poster B3

Fracture toughness of freestanding gold thin films studied by bulge testing — •Eva Preiss, Benoit Merle, and Mathias Göken — Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Materials Science & Engineering, Institute I, Germany

A versatile bulge test setup was used to perform mechanical tests on rectangular gold membranes with columnar microstructure and thicknesses ranging from 100 nm to 350 nm. It can be used in a conventional way to calculate stress-strain curves and determine parameters such as residual stress and plane-strain modulus. Alternatively, the setup can be inserted into an atomic force microscope (AFM) which allows in-situ imaging of the topography of the deforming membrane.

In order to determine the fracture toughness of thin films, narrow crack-like slits of 10 um length were milled into the center of the membranes by focused ion beam (FIB). Subsequently, the membranes were loaded until rupture.

The fracture toughness of all tested gold films is much lower than the literature value for bulk gold. However, the fracture toughness remains constant within the investigated thickness regime. In-situ AFM scans of the crack tip region show stable crack growth before failure. Plastic deformation is localized to a narrow corridor in front of the crack tip and mainly takes place along grain boundaries.

The obtained fracture toughness values agree well with literature values for other metallic thin films. New insights from the in-situ AFM scans are discussed with regard to possible deformation mechanisms.

MM 26.8 Tue 18:30 Poster B3

In situ micromechanical testing and local strain analysis of nanoporous gold — •Thomas Przybilla, Erich Thiess, Florian Niekiel, Benjamin Winter, Mirza Mačković, and Erdmann Spiecker — Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstrasse 6, 91058 Erlangen, Germany

Nanoporous gold (npg) acts as a model material to study mechanical size effects in nanostructured metals as the ligament size can be tailored within the nanometer to micrometer range. Au ligaments act together as a 3D open-porous network of interconnected nanostruts resulting in high mechanical strength under compression and nanoindentation. With decreasing ligament size stresses close to the theoretical shear strength were reported. In this work we study the mechanical behavior of npg foams with varying ligament diameter in the range of 10 to 100 nm by pillar compression experiments performed in situ via scanning electron microscopy (SEM) and transmission electron microscopy (TEM). npg pillars are prepared by focused ion beam (FIB) milling and characterized by scanning transmission electron microscopy (STEM) tomography. Taking the porosity into account the yield stress is evaluated with respect to the ligament diameter. The local strain is mapped from in situ experiments by image correlation techniques revealing local strain gradients and showing a distinct difference between local and macroscopic yield strain values.

MM 26.9 Tue 18:30 Poster B3

Plasticity of interfaces - TEM in situ indentation and atom probe microscopy on TiAl — •Carolin Puscholt and Mathias Göken — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Insitute I, Martensstr. 5, 91058 Erlangen, Deutschland

Interfaces in crystalline metallic materials significantly influence the material's mechanical properties. In fact, the study of the behavior of crystalline materials can often be reduced to the study of the structure and properties of their internal interfaces.

In this work Titanium Aluminides (Ti-48Al) are studied as a model system to determine the properties of interfaces since they offer a lamellar structure that represents a multilayer system made of two phases with a semi-coherent interface and a very distinct orientation relationship between the tetragonal γ-TiAl phase with its $L1_0$ structure and the hexagonal α_2-Ti_3Al phase with an ordered $D0_{19}$ structure. This was done by in situ indentation in the transmission electron microscope where the mechanical response of the material to indentation loads can be studied in real-time which permits the direct observation of the dynamics and mechanisms of dislocation motion and dislocation-interface interactions. Further investigations to study specific interface characteristics like segregations to (misfit) dislocations or deviations from the perfect stoichiometry of intermetallic phases that also strongly influence the properties were done via atom probe microscopy as a complementary method.

MM 26.10 Tue 18:30 Poster B3

Si diffusion and precipitation in Al during the Al-induced layer exchange (AlILE) process — •Simon M. Kraschewski, Benjamin Butz, and Erdmann Spiecker — Lehrstuhl für Mikro- und Nanostrukturforschung & Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg, Erlangen, Germany

Al-induced layer exchange (AlILE) is a promising route of fabrication for polycrystalline intrinsic Si seed layers from an amorphous state at low temperatures. The process makes use of the phenomenon of metal-induced crystallization and is characterized by a layer exchange in a stack of Si/oxide/Al on glass substrate at temperatures in the range of 180-550 °C. According to the current understanding of the process, atomic Si diffuses into the Al layer where it becomes oversaturated and forms crystalline precipitates. The precipitates grow laterally (up to several 10th of μm) thus replacing the Al which is "pushed up" into the original a-Si layer. Until now no analytical SEM/TEM studies have been performed in order to verify the Si content in the Al layer during the process.

First results on *ex situ* quenched samples with Si show a vertical gradient of Si in the Al layer with a range of 2-5 at%, which is much higher than expected from the phase diagram (round about 1 at%). Additionally the Si in the Al layer distribution seems to be independent from interfaces and grain boundaries.

MM 26.11 Tue 18:30 Poster B3

Electrochemical Hydrogenography on thin Magnesium films — •Niklas Teichmann, Magnus Hamm, Melissa Schenker, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany

Hydrogen in metals like Magnesium changes the physical properties of the host material, such as the optical properties.[1] This is the basic idea of the Hydrogenography where the change in the transistivity and reflectivity is measured to determine locally the Hydrogen concentration.[2] At room temperature the Mg-H system has a wide miscibiliy gap. This leads to a strong optical contrast.
In this paper, the optical change of thin Mg-films under hydrogen uptake is investigated using an electrochemical Hydrogenography technique.[3] By this, the MgH_2 formation can be measured and the formation kinetics can be studied.
As Mg oxidizes easily, oxides can be hardly prevented. In contact with hydrogen, hydroxides appear. These oxides and hydroxides directly influence the Hydrogen uptake and therefore, their impact is planned to be minimized.
Financial support by the DFG via projects PU131/9-2 and PU131/12-1 is gratefully acknowledged.
[1] T. Richardson et al. Applied Physics Letters 78.20 (2001): 3047-3049.
[2] R. Gremaud et al. Advanced Materials 19.19 (2007): 2813-2817.
[3] J. Kürschner et al. Journal of Alloys and Compounds 593 (2014): 87-92.

MM 26.12 Tue 18:30 Poster B3

Orientation changes upon attachment of spider hairs investigated in situ using scanning X-ray nanobeam

diffraction and small-angle scattering — •Silja Flenner[1], Clemens Schaber[2], Igor Krasnov[1], Stanislav Gorb[2], Christina Krywka[3], Emanuela Di Cola[4], Martin Rosenthal[4], Manfred Burghammer[4], and Martin Müller[1,3] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Institute of Zoology, Kiel University, Germany — [3]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany — [4]ESRF, Grenoble, France

The hairy attachment system of spiders enables these animals to walk upside-down on rough and smooth surfaces and support a multiple of the body weight without the use of glue. These outstanding biological structures comprise of pads including hundreds to thousands of specially designed hairs that are made of composite materials consisting of proteins and reinforcing chitin fibres.

The technique of high spatial resolution mapping based on scanning X-ray nanobeam diffraction and small-angle scattering was used to study the hairy attachment system of spiders. Each point of a map represents a structural parameter such as orientation or scattered intensity extracted from a diffraction pattern. This technique was combined with an in situ attachment/detachment procedure. The goal of our study is to gain an in-depth understanding of the working principle of the attachment and detachment processes of single hairs to a surface.

MM 26.13 Tue 18:30 Poster B3

X-ray Nanodiffraction for in situ Microscopy — •Christina Krywka[1,2], Stephan V. Roth[3], and Martin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht — [2]Christian-Albrechts-Universität, Leibnizstraße 19, D-24118 Kiel — [3]DESY, Notkestraße 85, D-22607 Hamburg

The origins of the macroscopic behavior of synthetic and natural high-performance materials can often be found on no less than atomistic length scales. Access to these dimensions is barred for light microscopes while electron microscopes suffer from the low penetration depth of electrons. Consequently, high resolution structural data recorded with external stimuli modified *in situ* is rare to find. X-ray nanodiffraction is able to overcome these hurdles. That's because a sub-micrometer sized hard X-ray beam can extract local structural information residing within bulk volumes and from samples inside extended sample environments - given a sufficiently long focal distance. The Nanofocus Endstation of P03 beamline (PETRA III) is a dedicated X-ray nanodiffraction setup. Tensile and indentation stresses, magnetic and electric fields, hydrostatic pressure and fluid shear have all been applied *in situ* in past nanodiffraction experiments at P03, i.e. while high resolution structural information data were recorded. Not only do these results emphasize our focus on materials science but they also demonstrate why X-ray Nanodiffraction is a genuine *in situ* microscopy technique.

MM 26.14 Tue 18:30 Poster B3

An Improved Method for Point Deflection Measurements on Rectangular Membranes — •Benoit Merle[1], Kyle Nicholson[1], Erik Herbert[2], and Mathias Göken[1] — [1]Materials Science & Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Materials Science & Engineering, Michigan Technological University, Houghton, USA

The point deflection method has recently emerged as a possible alternative to current micromechanical techniques for measuring the residual stress of thin films. A point deflection experiment consists into deflecting a clamped membrane in its center with a nanoindenter tip. The widespread availability of the required equipment makes the method very promising for future applications. These outlooks were further enhanced by the recent extension of the evaluation theory to rectangular membranes, which - unlike circular ones - are easily fabricated by standard lithographic techniques. In this work, the recent theoretical advances were critically reviewed and an improved experimental method based on the measurement of the contact stiffness was implemented. The new method was applied to the measurement of the residual stress of 100-nm thick SiNx and TiO2 membranes. The accuracy of the point deflection experiments was assessed by testing the same samples a second time with the bulge test reference technique. It is shown that the new experimental method dramatically improves the reproducibility of the measurements, and suggestions are made to improve the current evaluation scheme.

MM 26.15 Tue 18:30 Poster B3

Combining in situ tensile testing and orientation microscopy in the SEM: A MEMS based setup for studying the deformation of thin films — •Jan Philipp Liebig, Benoit Merle, and Mathias Göken — Institute I: General Materials Properties, FAU Erlangen-Nürnberg, Erlangen, Germany

Structures in integrated devices are constantly subjected to residual or thermal stresses during operation. Understanding the relaxation behavior of thin films is therefore critical for improving their reliability. Recently it was shown that Transmission Kikuchi Diffraction (TKD) in the SEM enables the determination of local crystal orientations with high spatial resolution using standard Electron Backscatter Diffraction instrumentation [1]. Giving access to quantitative information on mechanisms like grain growth, grain rotation and strain gradient evolution, time resolved TKD stands out as a promising technique for the characterization of microstructural changes upon relaxation of thin films. We have implemented a MEMS based tensile device [2] into a custom setup specifically designed for in situ TKD imaging inside the SEM. A scanning TEM detector is used complementarily to access shorter time scales. In this context, a novel technique for the preparation and mounting of freestanding thin film tensile samples is presented, which relies on focused ion beam (FIB) milling and selective, electron-beam-assisted etching of silicon membranes.

[1] R.R. Keller, R.H. Geiss, J. Microsc. 245 (2012) 245.
[2] E. Hosseinian, O.N. Pierron, Nanoscale 5 (2013) 12532.

MM 26.16 Tue 18:30 Poster B3

In-operando soft x-ray microspectroscopy of organic field-effect transistors — •Xiaoyan Du, Benedikt Rösner, and Rainer Fink — Physikalische Chemie II, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany

Organic semiconducting films bear high potential for organic electronics. While many studies are devoted to the morphology and interface of the semiconducting thin film, investigations of the devices under operation are rather scarce. Microscopic resolution further allows to correlating film morphology with charge transport. Upon application of gate and/or source-drain voltages in organic field-effect transistors (OFETs), the energetic levels of organic semiconductor shift enabling charge accumulation and charge transport. In-operando NEXAFS spectroscopy in Scanning Transmission X-ray Microspectroscopy (STXM) were used to study the density of unoccupied density of states (UDOS). In order to correlate the impact of external fields (gate effect) to energetic shifts of the occupied levels (HOMO, core levels), spatially resolved XPS measurements were explored. In this contribution, we discuss various aspects and limitations of in-operando microspectroscopy using α, ω-dihexyl-sexithiophene (DH6T) based OFETs to obtain full insight into the electronic structure.

MM 26.17 Tue 18:30 Poster B3

Fabrication and application of static liquid cells for transmission electron microscopy — •Andreas Hutzler[1], Robert Branscheid[2], Benjamin Butz[2], Michael P. M. Jank[3], Lothar Frey[1,3], and Erdmann Spiecker[2] — [1]Chair of Electron Devices, FAU Erlangen-Nuremberg, Germany — [2]Center for Nanoanalysis and Electron Microscopy, FAU Erlangen-Nuremberg, Germany — [3]Fraunhofer Institute for Integrated Systems and Device Technology, Germany

In situ liquid cell transmission electron microscopy (LCTEM) is a highly attractive characterization method for nanoparticle systems, because it enables real time imaging in liquid environment under the high vacuum requirements of electron microscopy. In our approach we present the batch fabrication of custom-designed static liquid cells for conventional specimen holders adapted to the design of Zheng et al. [1]. The basic concept is to confine a fluid in a channel between two electron-transparent membranes enclosed by a silicon frame which is structured by micromachining. Experimentally we could demonstrate growth and degradation processes of Au nano-rods induced by electron beam irradiation. While further development of functionalized cells is ongoing, our aim is the study of various material processes under liquid conditions as well as the enhancement of the LCTEM methodology itself. E.g. radiation damage and resulting secondary effects have not been investigated systematically to date although they have been observed in numerous studies.

[1] H. Zheng et al., Science 2009, **324**, 1309–1312

MM 26.18 Tue 18:30 Poster B3

Electrical Conduction in Thin Layers of ZnO Nanoparticles, Studied Under Various Conditions — •Moses Richter, Jo-

hannes C. Voll, Gebhard J. Matt, Michael Salvador, and Christoph J. Brabec — i-MEET, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91058 Erlangen, Germany

Solution cast thin layers of nanoparticles are important to many novel printed electronics, e.g. organic solar cells, organic LEDs and OFETs. However, stable ink formulations require the use of stabilizing ligands, which strongly influence the electrical conduction in the dried layer, hence the device performance. The limiting conduction mechanism in aforementioned layers is identified in low temperature experiments as a Poole-Frenkel limited transport. By in-situ UV-light treatments under various atmospheric conditions, the responsible defects could be correlated to the particle surfaces. The actual electronic change in UV-light treated ZnO layers is further evaluated by Kelvin Probe-AFM scans and the influence on organic solar cell performance. In latter it turned out to improve the long time stability and maximal achievable performance.

MM 26.19 Tue 18:30 Poster B3

Probing the dynamics of piezoelectric field in GaN nanorods by in-situ bending in transmission electron microscope with differential phase contrast and electron diffraction mapping — •Mingjian Wu[1], Florian Niekiel[1], Christel Dieker[1], Silke Christiansen[2], and Erdmann Spiecker[1] — [1]WW9 & CENEM, Department Werkstoffwissenschaften, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany — [2]MPI for the Science of Light, Günther-Scharowski-Str. 1, 91058 Erlangen, Germany

Probing the electric properties of functional semiconductors in nanoscale resolution is of great interest, because it allows direct visualization of the relation to the local structure and especially defects. Inversion domain boundary (IDB) is one of the common defects found in wurtzite GaN, a polar crystal with piezoelectricity. As is known, piezoelectricity couples to the polarity of crystal and the sign of applied stresses. For wurtzite GaN nanorods with IDB upon mechanical bending, the piezoelectric field and charge distribution would be expected to be greatly different to normal GaN nanorods. Experimentally, electric fields can be visualized down to atomic scale, in principle, by the deflection of electron probe (i.e., differential phase contrast (DPC)). In this work, we perform in-situ mechnical bending of GaN nanorods with side-to-side IDB in the TEM, and acquire DPC micrographs and convergent beam electron diffraction pattern arrays to infer the dynamics of piezoelectric field in the GaN nanorods. Interesting findings and comprehensive data evaluation and interpretation will be presented.

MM 26.20 Tue 18:30 Poster B3

Investigating the formation, growth and phase transition of semiconductor nano-crystals in solid by in-situ annealing in TEM — •Mingjian Wu[1,2,3], Esperanza Luna[2], Janne Puustinen[3], Mircea Guina[3], Achim Trampert[2], and Erdmann Spiecker[1] — [1]WW9 & CENEM, Department Werkstoffwissenschaften, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany — [2]Paul-Drude-Institut, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [3]Optoelectronics Research Centre, Tampere University of Technology, PO Box 692, 33101, Tampere, Finland

Spontaneous formation of semiconductor nano-crystals in solids is of technological importance and of great scientific interest. It can be driven by the intrinsic tendency to phase separation of metastable compounds, if the atomic diffusion is activated. The controllability of the resulting structure and phase relies on a deeper insight into the atomic diffusion process and defects interaction. This can be scoped by observing individual events and/or from statistics of their time and temperature dependency, which is missing in ex-situ studies. Recently, we observed ex-situ, upon annealing, the formation and phase transformation of Bi-containing nano-crystals embedded in GaAs matrix, which might in principle operate as quantum dots. In this work, we perform in-situ annealing experiments on dedicated Ga(As,Bi) epilayers in the TEM. The dynamics of formation and growth of Bi-containing nano-crystals is revealed; and even their phase transformation and interaction with dislocation loops is observed. We will present the latest results and a comprehensive evaluation and interpretation of the data.

MM 26.21 Tue 18:30 Poster B3

In situ TEM Interfacial Electrochemistry of Fluoride Ion Batteries — Mohammed Hammad[1,2], •Mohammad Saleh Gorji[1,2], Venkata Sai Kiran Chakravadhanula[1,2,3,4], M. Anji Reddy[1,3], Carine Rongeat[1], Torsten Scherer[1,4], Horst Hahn[1,2,3], Maximilian Fichtner[1,3], and Christian Kübel[1,3,4] — [1]INT, Karlsruhe Institute of Technology (KIT), Germany — [2]TU Darmstadt, Germany — [3]HIU, KIT, Germany — [4]KNMF, KIT, Germany

In situ transmission electron spectroscopy provides high spatial resolution visualization of battery operations in real time, giving an important insight on the electrochemistry of batteries. Fluoride ion batteries have a great potential to be an alternative to the conventional Li ion batteries because of the high electronegativity and comparable low atomic weight of the fluorine. In this study, the structural properties of a micron-sized all-solid-state fluoride ion battery at the interfaces between electrolyte and electrodes, and their degradation mechanisms during cycling, have been investigated by in-situ TEM. Ball milling was used to prepare the La0.9Ba0.1F2.9 electrolyte and the cathode was a composite of Cu and C and the anode a composite of MgF2, Mg, La0.9Ba0.1F2.9 and C. The battery was cycled between 0 V to 3.5 V. HRTEM micrographs revealed the formation of CuF2. Additionally, morphological changes observed at the interfaces are presented.

MM 26.22 Tue 18:30 Poster B3

New approach of segmentation of FIB tomograms of porous carbon-rich materials — •Manuel Mundszinger, Jörg Bernhard, Ute Golla-Schindler, and Ute Kaiser — Ulm University, Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Focused ion beam (FIB)-Tomography is widely used in material sciences to gain quantitative information about the topography and composition of the specimen under investigation. With a single tomogram it is possible to determine the volume fraction and the surface of a selected element. Segmentation of FIB tomograms of a porous material can, however, be very troublesome caused by the high depth of focus given by the scanning electron microscope. Thus, the same grey level can be obtained e.g. for the top and the bottom of a pore. This can become the restricting hurdle for a reliable segmentation of the single picture and therefore of the whole tomogram. One possibility is to fill the pores with resin to decrease the insights in the sample structure. However, many resins are carbon-based and therefore this procedure only works fine as long as the sample does not contain carbon. Here we present a new way to face the problem associated with FIB-tomograms of porous materials with carbon-rich inclusions. For our method we use carbon-free industrial available coatings to avoid the loss of the carbon contrast in the SEM images. The best results were obtained when the sample was hydrophilized using a plasma cleaner, which increased the wetting and therefore the pore filling of the sample greatly.

MM 26.23 Tue 18:30 Poster B3

Towards Conductivity Measurements in Battery Materials Using Scanning Electron Microscopy — •Sebastian Sturn, Ute Golla-Schindler, Jörg Bernhard, and Ute Kaiser — Electron Microscopy Group, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

There are several ways of determining the conductivity of bulk materials, especially known in the field of solid state physics. However, the experiments will usually yield only the mean conductivity. We try to spatially resolute the electrical conductivity of state-of-the-art secondary battery electrodes by means of injecting electrons using an SEM.

In a first step, it is necessary to determine the amount of incident electrons absorbed in the bulk material. It is therefore crucial to quantitatively characterize any electron current exiting the specimen, namely the secondary electron and backscattered electron current, since the absorbed current is given by $I_{abs} = I_{incident} - I_{SE} - I_{BSE}$.

The approach is to directly measure I_{SE} and I_{BSE} for every spot of the scan pattern. By using Focused Ion Beam (FIB), we are able to get rid of the specimen's topography and prepare polished surfaces. As the secondary electron yield is mainly dependent on the topography, we are able to, at least as a first approximation, assume that the secondary electron current is constant.

The use of a Gas Injection System (GIS) allows for sputtering platinum contacts on top of the specimens. We use these platinum pads as contact areas for micromanipulators to read out absorbed currents.

MM 26.24 Tue 18:30 Poster B3

Interaction of hydrodynamic cavitation bubbles with textile linen in an open reactor — Patrick Casper, Tamara Neumann-Schmidt, •Florian Szillat, Hans-Günter Hloch, and Jürgen Bohnen — wfk - Cleaning Technology Institute, D-47807 Krefeld, Deutschland

The amount of individually and fashionably Corporate Identity clothing is increasing in hygienically demanding areas. During reprocessing of such clothing, extensive hygiene measures have to be fulfilled. Meeting high demands on non-destructive textile processing and sustainability as well as hygiene requirements, the use of hydrodynamic cavitation is of great interest, as it is providing mechanical impact and reactive oxygen species under textile preserving conditions. Recent studies (e.g. [1]) demonstrated the capability of hydrodynamic cavitation in the field of pharmaceuticals/chemicals degradation. These systems are based on venturi nozzle or orifice plate design in closed tubular systems, whereas an open environment is necessary for reprocessing of clothing. To obtain a better understanding of behaviour of hydrodynamic cavitation bubbles outside of nozzles and such tubular systems their distribution in an open reactor is studied using luminescence. Furthermore, interplay of parameters and nozzle design is investigated by means of dye destruction analysis. Implications of bleaching and disinfection as well as influence of design and parameters on the use of hydrodynamic cavitation at water-textile interfaces will be discussed.

[1] P. Braeutigam et al. Water Research 46 (2012) 2469

MM 26.25 Tue 18:30 Poster B3

Mechanical properties of 3D printed polymers on textile fabrics with interface layer modification — •Nils Grimmelsmann[1], Mirja Lutz[2], Michael Korger[2], Hubert Meissner[1], and Andrea Ehrmann[1] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld, Germany — [2]Niederrhein University of Applied Sciences, Mönchengladbach, Germany

Composites produced from two or more different materials with different physical and chemical properties often allow for tailoring mechanical and other characteristics of the resulting multi-material system. Fiber-reinforced plastic composites have usually high strength and elasticity due to a combination of the tough but weak plastic matrix with the strong and stiff reinforcing fibers, filaments or textile layers.

Combinations of textile materials with 3D printed polymers, however, result in different mechanical properties of the composites. While the tensile strength of the multi-material system is increased compared to the pure 3D printed material, the elasticity of the polymer layer can be retained to a certain degree, since the textile material is not completely immersed in the polymer. Instead an interface layer is built in which both materials interpenetrate to a certain degree.

The poster will give an overview of the parameters affecting the interface layer. The influence of this interface layer on possible delamination and mechanical properties of the developed composites will be depicted, resulting in the possibility to tailor the desired strength and elasticity of polymer-textile composites.

MM 26.26 Tue 18:30 Poster B3

Synthesis and electrochemical properties of orthorhombic α-MoO_3 and hexagonal h-MoO_3 nanostructures — •Christina Schmidt[1], Alexander Ottmann[1], Galina Zakharova[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, Germany — [2]Institute of Solid State Chemistry, Ural Division, Russian Academy of Sciences, Yekaterinburg, Russia

MoO_3 nanomaterials with either hexagonal or orthorhombic crystal structure have been synthesised by means of a microwave-assisted hydrothermal route. The different structures are obtained by varying the synthesis parameters, which also leads to different size and shape of the primary particles. Magnetisation studies by means of SQUID magnetometry allow assessing that less than 0.1 % of Mo^{5+}-defects are present in the materials. The electrochemical properties of the different samples are studied by means of cyclic voltammetry and galvanostatic cycling, and are discussed with regard to the XRD, SEM and SQUID data. Cyclic voltammetry reveals reversible processes associated with the Mo^{6+}/Mo^{5+} redox couple in the α-MoO_3 nanostructures. Galvanostatic cycling within the potential limits of 1.5-3.5 V vs. Li/Li^+ of α-MoO_3 nanorods shows an initial discharge capacity of 296 mA h g^{-1} at 100 mA g^{-1}. In case of h-MoO_3 nanostructures, except for large irreversible initial effects, only low electrochemical activity is observed.

MM 26.27 Tue 18:30 Poster B3

Doping studies and structural, magnetic, and electrochemical characterization of tetrahedral $LiCo_{1-x}M_xPO_4$ (M = Cu, Fe, Zn, Y) — •Yuquan Wu[1], Verena Neder[1], Benjamin Herdeanu[1], Lucas Schlestein[1], Hans-Peter Meyer[2], Christoph Neef[1], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Institut für Geowissenschaften, Heidelberg University, D-69120 Heidelberg, Germany

Tetrahedral $LiCo_{1-x}M_xPO_4$ microstructures with transition metals M such as Cu, Fe, Zn, and Y are synthesized by a microwave-assisted hydrothermal method. For each dopant, the accessible doping range x is studied and the effect of doping on the crystal structure as well as on the morphology is investigated. Non-magnetic Zn-doping allows investigating the slightly diluted magnetic system $LiCo_{1-x}Zn_xPO_4$ with x 0.05, as well as paramagnetic $LiCo_{0.05}Zn_{0.95}PO_4$ which enables studying well separated magnetic Co-centers. Regarding the electrochemical behavior, low doping levels enhance the intercalation kinetics while high doping levels yield a clear reduction of electrochemical capacity as demonstrated by cyclic voltammetry. In contrast to well known olivine-like $LiFePO_4$, the iron doped tetrahedral structure shows no appreciable electrochemical activity that can be clearly associated with the Fe^{2+}/Fe^{3+} redox couple.

MM 26.28 Tue 18:30 Poster B3

Hydrogen treatment of $Fe_{60}Al_{40}$ thin films — •Jonathan Ehrler[1,2], Rantej Bali[1], Camilo Otalora[1], Wolfgang Anwand[1], Roman Böttger[1], Maciej O. Liedke[1], Thomas G. Woodcock[3], and Kay Potzger[1] — [1]HZDR, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Dresden University of Technology, Helmholtzstrasse 10, 01069 Dresden, Germany — [3]IFW Dresden, PO Box 270116, 01171 Dresden, Germany

The effect of H treatment on the magnetic properties and the defect concentration of $Fe_{60}Al_{40}$ films, possessing A2 and B2 structure respectively, have been investigated. The treatment was realized by H^+ irradiation as well as by reactor loading. Ferromagnetic A2-$Fe_{60}Al_{40}$ films of 250 nm thickness were irradiated with protons at an energy of 17 keV and fluences of up to 1.46 E18 ions cm^{-2}. Magneto-optical Kerr effect showed a variation of coercivity and an increase of saturation magnetization (M_S) as a function of ion fluence. Positron annihilation spectroscopy (PAS) indicates an increase of the open volume defect concentration. Superparamagnetic B2-$Fe_{60}Al_{40}$ films were annealed at 423 K in 30 bar H atmosphere. PAS shows that the H-annealing process led to a decrease in the open volume defect concentration. H-treatment caused a small increase in M_S from 0.013 to 0.017 μ_b/Fe atom, as well as a shift in the blocking temperature from 85 to 115 K respectively. While H treatment significantly modifies the magnetic properties of $Fe_{60}Al_{40}$, elastic recoil detection suggests that the hydrogen is not retained in the vacancies present in the film, suggesting that the variations may be mostly due to structural changes.

MM 26.29 Tue 18:30 Poster B3

Mg2Fe(x)Si(1-x) - hydride: The interplay between, defects, structure and magnetic properties — •Thu Trang Trinh[1,2], Oguz Yildirim[1], Oskar Liedke[1], Wolfgang Anwand[1], Andreas Wagner[1], Kohta Asano[3], Bernard Dam[4], and Kay Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Dresden University of Technology, Helmholtzstrasse 10, 01069 Dresden, Germany — [3]Energy Technology Research Institute, Ibaraki 305-8565, Japan — [4]Delft University of Technology, 2628 BL Delft, Netherlands

Mg2Fe hydride belongs to the most promising candidates for application as light weight storage material in a future hydrogen economy. Recently, it has also been shown that due to chemochromism, Mg2Fe is a low-cost and rare-earth-free candidate for switchable mirrors upon hydrogen loading. Besides the Mg2Fe hydride, a new compound of Mg2(FeSi) will be presented. The additional content of Si promises an optimization of hydrogen absorption and desorption processes. The Fe component of the system makes it an interesting material in terms of magnetic applications. Comprehensive investigations on Mg2(FeSi) system showed that hydrogen induced changes in structure, electronic, optical and magnetic properties. E g., volume magnetic properties transform from superparamagnetism to ferromagnetism with a high Curie temperature. In order to understand the basic physical properties of Mg2(FeSi) thin films and its hydride the present studies involve fundamental research and defect analysis.

MM 26.30 Tue 18:30 Poster B3

Thermal decomposition of sodium borohydride covered with polyethyleneimine — •Hendrik Rahmann[1], Christian Sternemann[1], Sebastian Dahle[2], Georgia Sourkouni[2], Christos Argirusis[2,3], Karin Esch[1], Florian Wirkert[1], Holger Göhring[1], Wolfgang Maus-Friedrichs[2], and Metin Tolan[1] —

[1]Twchnische Dortmund, 44221 Dortmund, Germany — [2]Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany — [3]National Technical University of Athens, 15773 Zografou/Athens, Greece

In order to use hydrogen as an energy carrier in the future as part of real-life technologies, efficient hydrogen storage media are necessary. Borohydrides are an attractive hydrogen storage material because of their low mass and high hydrogen density. Here, one of the promising candidates is sodium borohydride ($NaBH_4$) if its degradation at atmosphere can be hindered and its hydrogen release temperature can be lowered. To achieve this goal, $NaBH_4$ can be covered with a polyethyleneimine (PEI) layer [1]. We performed in situ X-ray diffraction (XRD) measurements at beamline BL9 of DELTA synchrotron radiation source using native and PEI-coated $NaBH_4$ while heating the samples from 30°C to 720°C. The crystalline reaction products at different temperatures were determined in order to compare both hydrogen release paths. Moreover we applied quadrupole mass spectrometry and differential scanning calorimetry to characterize changes in the hydrogen desorption path of $NaBH_4$ induced by PEI coverage.

[1] S. Dahle et al., RSC Adv. 4, 2628 (2014).

MM 26.31 Tue 18:30 Poster B3

Materials for all solid-state thin-film batteries — •Susann Nowak[1], Priyanka Sharma[1], Giulio Calcagno[1], Matthias Köhler[2], Juliane Mürter[1], Fabian Wunde[2], and Guido Schmitz[1] — [1]Heisenbergstr. 3, 70569 Stuttgart — [2]Wilhelm-Klemm-Str. 10, 48149 Münster

All solid-state batteries received increasing attention over the last years due to the simplified packaging process and increased energy density and safety. The defined thin-film geometry is also well suited to conduct fundamental studies of thermodynamics and kinetics of batteries. Since batteries are complex multilayer devices, it is essential to optimize and characterize anode, cathode and electrolyte materials carefully before combining them in an all solid-state battery. This contribution presents a wide construction-kit of different battery materials which can be successfully produced by ion-beam sputtering. In particular the fabrication and properties of LFP, LMO, LCO, NMC, Sn, Si and LiPON as thin films are shown. Challenges of balancing a full cell and its effects on the energy density of a battery are discussed on a LFP-Sn anode-cathode model. First results on combining battery materials are shown. The behavior of the storage materials can vary drastically due to differing interfacial properties.

MM 26.32 Tue 18:30 Poster B3

Deposition of transition metal oxide thin film cathode materials for Li-ion battery application — •Geoffrey Matthew Tan[1], Christoph Loho[1], Oliver Clemens[1,2], and Horst Hahn[1,2,3] — [1]Joint Research Laboratory Nanomaterials, Darmstadt, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]Helmholtz Institute Ulm, Ulm, Germany

The development of smaller and more powerful electronic devices places a strong demand on energy sources that are compact, safe and have a high energy density. Solid state thin film lithium ion batteries are one of the candidates to fulfill this demand. The use of aerosol assisted chemical vapor deposition (AA-CVD) to precisely control stoichiometry in nickel substituted LiCoO2, which acts as cathode in such a device, is a possible strategy to increase the energy density.

The aim of this study was to find the optimum process parameters for LiCoO2 thin film deposition using AA-CVD and to substitute cobalt by nickel to form lithium nickel cobalt oxide, because of its higher energy density and lower cost.

The structure, morphology and phase composition of LiCoO2 films as well as nickel substituted films were studied comprehensively. Phase pure LiCoO2 was deposited at 850 °C. Electrochemical characterization in a Swagelok type half-cell demonstrated a specific capacity of 94 mAh/g for LiCoO2. Despite the precise control of the nickel to cobalt ratio, the deposited thin films do not show the desired phase. Their electrochemical activity will be discussed.

MM 26.33 Tue 18:30 Poster B3

Surface Excess Elasticity: A First-Principles Study — •Beatrix Elsner and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 HH

The size-dependent elastic response of nanomaterials and nanostructures with a large surface-to-volume ratio has attracted increasing attention. Yet, it remains an open question whether the presence of surfaces entails a stiffening or softening of the material [1]. The surface elastic constants–a measure for the change of surface stress with surface strain–represent a key quantity with regard to this question. In this contribution, we present a density functional theory (DFT) study of the surface energy, surface stress, and surface elastic constants of low-index fcc metal surfaces. Our calculations yield positive surface elastic constants for the (111) and (001) surfaces of gold, implying a stiffening effect.

Supported by DFG, SFB 986, project B3.

[1] Mameka, et al., Acta Materialia **76**, 272 (2014).

MM 26.34 Tue 18:30 Poster B3

Quantum mechanically based prediction of surface segregation in Ag-Au alloys — •Sandra Hoppe and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (npAu) offers a high catalytic activity for certain chemical reactions combined with a high selectivity. This phenomenon can theoretically be explained in two ways: First, the rough morphology provides a large number of low-coordinated Au atoms. Second, Ag impurities remaining from the dealloying process may supply reaction sites. Interestingly, Au (111) surfaces roughened by sputtering have been found inactive towards CO-oxidation [1]. Previous density functional theory (DFT) results imply that Ag impurities in the surface dissociate molecular O_2 and supply O atoms [2]. Experimental results show that the catalytic activity of npAu can be tailored via the residual Ag concentration. The aim of this work is to characterize clean Ag-Au surfaces regarding their segregation profile. DFT calculations serve as input for a surface cluster expansion (CE). We find that the resulting surface composition depends strongly on the applied exchange correlation functional. To obtain Ag enrichment in the surface layer, as it has been observed in experimental and theoretical studies [3], it seems necessary that both the lattice parameters and the surface energies of the pure elements are calculated in the correct hierarchy.

[1] J. Gong *et al.. J. Phys. Chem. C* **112** (2008) 5501.
[2] L. V. Moskaleva *et al.. Phys. Chem. Chem. Phys.* **13** (2011) 4529.
[3] e.g. T. Déronzier *et al.. J. Catal.* **311** (2014) 221.

MM 26.35 Tue 18:30 Poster B3

The formation of nc-Si in SiOx induced by continuous-wave laser irradiation — •Nan Wang[1], Thomas Fricke-Begemann[2], Patrick Peretzki[1], Michael Seibt[1], and Jürgen Ihlemann[2] — [1]IV. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Laser-Laboratorium Göttingen, Hans-Adolf-Krebs-Weg 1, 37077 Göttingen, Germany

Silicon nanocrystals embedded in substoichiometric SiOx (silicon-rich silicon oxide) exhibit room-temperature photoluminescence due to quantum confinements. The generation of nc-Si can be induced by thermal annealing or laser irradiation. It is known that laser irradiation on free-standing SiOx without substrate may avoid the heat flow into the substrate. Here we employ continuous-wave laser irradiation at 405 nm wavelength to focus a 6 μm diameter spot on 545 nm thick SiOx films deposited on fused silica substrates. A high density of nc-Si particles is obtained. The samples are characterized by AFM, TEM, Raman spectroscopy and photoluminescence. The spatial distribution of the nanocrystals in the irradiated area is determined. At a laser irradiance of $1.2{\cdot}10^5$ W/cm^2, an almost perfect damage-free irradiation is obtained. At higher laser power the central region exhibits some porous properties, and the nc-Si region is located beneath the porous region. In summary, we have demonstrated that laser annealing offers the possibility to generate Si nanoparticles in a fast, high throughput process. Also, the thermal load on the substrate can be significantly reduced.

MM 26.36 Tue 18:30 Poster B3

Synthesis and characterization of bulk heterojunction solar cells based on nanoporous templates — •Sven Hilke[1], Yonggang Zhen[2], Wenping Hu[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Chemistry, Chinese Academy of Sciences, ZhongGuanCun North First St 2, Beijing 100190, P. R. China

The well-known system Zn-Phthalocyanine:Fullerene (ZnPc:C60) as a model system of bulk-heterojunction solar cells has been chosen to analyze the effect of a nanoporous structuring on the applicability of the resulting hetero molecular mixture. In this context, the basis of the

pre-structuring is an Anodic Aluminum Oxide (AAO) membrane made of aluminum oxide constructed by electrochemical processes. The controlled wet-chemical deposition via the dipNdry (dipping and drying) method generates tubes or rods (depending on concentration, solvent as well as dipping time and repetition). Naturally, the pre-structuring directly influences the morphology on the nanometer scale. The presented work consists of the controlled growth of the nanoporous templates to obtain regular pore structures with equal and uniformly distributed surface area in the hetero intersection. In addition, every single nanopore is individually functional so that the failure of a single nanopore does not cause the destruction of the whole solar cell. Scanning electron and scanning tunneling microscopy, as well as optical characterizations are used to analyze the obtained structures.

MM 26.37 Tue 18:30 Poster B3

Computational design of metal-organic frameworks with paddlewheel-type secondary building units — •Udo Schwingenschögl, Maxim V. Peskov, and Nejib Masghouni — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

We employ the TOPOS package to study 697 coordination polymers containing paddlewheel-type secondary building units. The underlying nets are analyzed and 3 novel nets are chosen as potential topologies for paddlewheel-type metal organic frameworks (MOFs). Dicarboxylate linkers are used to build basic structures for novel isoreticular MOF series, aiming at relatively compact structures with a low number of atoms per unit cell. The structures are optimized using density functional theory. Afterwards the Grand Canonical Monte Carlo approach is employed to generate adsorption isotherms for CO_2, CO, and CH_4 molecules. We utilize the universal forcefield for simulating the interaction between the molecules and hosting MOF. The diffusion behavior of the molecules inside the MOFs is analyzed by molecular dynamics simulations.

MM 26.38 Tue 18:30 Poster B3

A new method for synthesis of graphite oxide nanoplatelets from bamboo pyroligneous acid: Morphological, structural and transport properties — •Katherine Gross[1], Jhon J. Prias[2,3], Soraya Sangiao[4], Jose M. DeTeresa[4], Hernando Ariza[2], and Pedro Prieto[1] — [1]CENM, Universidad del Valle, Colombia — [2]IIS, Universidad del Quindío, Colombia — [3]EITP, Universidad del Quindío, Colombia — [4]LMA, INA Universidad de Zaragoza, Spain

In this work we present a new and cost-effective method for the synthesis of graphite oxide nanoplatelets (GONP) using bamboo pyroligneous acid (BPA) as source.Characterization by Raman, FTIR and XRD techniques confirm that increased carbonization temperature increases graphite conversion. GONP-BPA present lateral dimensions of 5-100×10^3 nm and thickness less than 80 nm. HRTEM and EEL spectra reveal that locally the carbon is mainly in sp2 bonding configuration and confirm a short/medium range of crystalline order. For electrical characterization, single nanoplatelets were contacted by focused-ion-beam-induced deposition of Pt nanowires. The electrical conductivity at room temperature shows a rise of three orders of magnitude by reducing the atomic percentage of oxygen from 17 to 5 percent, reaching a final value of 2.3×10^3 S/m. Temperature-dependent conductivity measurements show a semiconductor-like behavior with weak temperature dependence. This research shows that BPA can be used for sustainable creation of graphitic carbon which could be used in the development of advanced devices.

MM 26.39 Tue 18:30 Poster B3

Comparison of nanoparticles in printer toners between original equipment manufacturer to office supplies manufacturer — •Paula Weber, Miriam Leifels, and Mathias Getzlaff — Heinrich-Heine-Universität Düsseldorf

We use laser printer toners in our everyday life. To identify its composition and the material properties we must examine it at the nanoscale. So we can, for example, observe a lot of different nanoparticles in printer toners. The differences between the various printer toner manufacturers in terms of nanoparticles relating to the size, the element composition as well as the various physical properties are remarkably.

This contribution will exemplarily discuss the comparison between the printer toner of original equipment manufacturer and the printer toner of office supplies manufacturer.

Different experimental techniques make the comparison possible. These include Dynamic Light Scattering (DLS), X-Ray Diffraction (XRD), Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM) and Energy Dispersive X-Ray Spectroscopy (EDX).

The sizes can be measured by DLS and electron microscopy. XRD allows to obtain information on the structure of the nanoparticles. The remaining questions can be answered by a specific SEM with integrated EDX.

By comparing the results of the various above mentioned methods, we get knowledge concerning the used nanoparticles.

Finally, the nanoparticles of the two different manufacturers are compared with each other to determine the similarities and differences.

MM 26.40 Tue 18:30 Poster B3

Oxygen vacancy diffusion in sodium bismuth titanate studied by density functional theory calculations — •Kai-Christian Meyer, Melanie Gröting, and Karsten Albe — TU Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

Sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$, NBT) is a ferroelectric relaxor-like material at room temperature and has interesting electrical properties for application as a high strain actuator material. It shows a broad diffuse phase transition from a ferroelectric (rhombohedral/monoclinic) structure to a weakly polar (tetragonal) state. Recently, it has been shown that doped NBT exhibits a high ion conductivity, in contrast to other perovskites. [1] Thus, in this work we investigate by means of density functional theory calculations oxygen vacancy formation energies, association energies with different metal ions and migration barriers for different A-cation orders. We find among other things that the chemical order plays a strong role on the atomistic level, eg. for local phase transitions [2] and conductivity.

[1] M. Li, *et al.*, Nat. Mater. 13, 31 - 36 (2014)

[2] K.-C. Meyer, *et al.*, J. Solid State Chem. 227, 117 - 122 (2015)

MM 26.41 Tue 18:30 Poster B3

Nonequilibrium Dynamics of the spin system and lattice heat in the rare earth Dysprosium — •Alexander von Reppert[1], Jan Pudell[1], Karine Dumesnil[2], Flavio Zamponi[1], and Matias Bargheer[1,3] — [1]Institut für Physik und Astronomie, Potsdam, Germany — [2]Institut Jean Lamour, Vandoeuvre les Nancy cédex, France — [3]Helmholtz Zentrum Berlin, Berlin, Germany

We present a temperature and fluence dependent Ultrafast X-Ray Diffraction study of a laser-heated Dysprosium thin film. A pronounced lattice contraction heralds the ultrafast loss of antiferromagnetic order, which is reestablished on a nanosecond timescale when the heat reservoir of the phonons in Dy has cooled well below the Néel temperature. The calibration of the position and width of the Bragg peaks in thermal equilibrium allows for a detailed experimental measurement of the energy deposited in the lattice and spin system. Reestablishing the magnetic order by cooling of the magnetic system is much slower than cooling the lattice, especially around the Néel temperature. Although the system shows very strong magnetostriction, the transfer of energy from the spin system to the lattice is weak after the spin-order is lost.

MM 26.42 Tue 18:30 Poster B3

In situ microscopy of material transport and Ge crystallization in the Al-induced layer exchange (ALILE) process — •Janis Wirth, Simon M. Kraschewski, and Erdmann Spiecker — Lehrstuhl für Mikro- und Nanostrukturforschung und Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg, Erlangen, Germany

The Al-induced layer exchange (AlILE) process exploits the phenomenon of metal-induced crystallization to fabricate polycrystalline seed layers of Si or Ge at low temperatures [1, 2]. In order to understand the process and the material transport involved we use a combination of different in situ microscopy techniques. At low magnification in situ light microscopy reveals the nucleation and growth of crystalline nuclei as well as the overall kinetics of the process. At higher magnification in situ STEM is employed for studying the details of material transport at and near the crystallization front. Due to the small difference in atomic numbers of Al and Si, the Si-ALILE process cannot be directly visualized by Z-contrast imaging. Using Ge instead of Si, Z-contrast imaging benefits from the considerably larger difference in the atomic number. Similar to Si-AlILE, the Ge-AlILE process is characterized by a layer exchange using a stack of a-Ge/AlO_x/Al on glass or SiN_x substrate at temperatures of 220-417°C. Ge diffuses into the Al layer and forms crystalline precipitates upon supersaturation. Subsequently the precipitates grow while the Al is pushed up into the a-Ge top layer.

[1] J. Schneider et al., J. Non-Cryst. Solids 352, (2006)

[2] K. Nakazawa et al., J. Solid State Science 2 (2013)

MM 26.43 Tue 18:30 Poster B3

Local measurement of stress-strain-curves by spherical nanoindentation — •Patrick S. Feldner, Benoit Merle, and Mathias Göken — Materials Science and Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU)

In contrast to sharp indenters, spherical indenters offer the possibility to determine continuously the stress-strain response of a material at a very local scale. However due to the complex deformation field, various approaches are available for approximating the stress and strain during spherical nanoindentation experiments, leading to significantly different evaluations of the yield behavior of the material.

The aim of this work was to establish a reliable analysis procedure to turn nanoindentation raw data into meaningful stress-strain-curves. This procedure was further extended to the development of a new method for determining the strain-rate sensitivity of flow stress as a function of strain. In the case of ultrafine-grained metallic materials, it is shown that this information in combination with other micromechanical and structural characterization methods, could give new insights into the evolution of the different deformation mechanisms in dependence of the imposed strain.