MM 27: Poster Session I

Time: Tuesday 18:30–19:45 Location: Poster E

MM 27.1 Tue 18:30 Poster E

Quantitative mapping of transient fields in plasmonic devices employing a novel STEM technique — •Johannes Schultz[1], Jonas Krehl[1], Axel Lubk[1], Darius Pohl[2], Giulio Guzzinati[3], Jo Verbeeck[3], and Tobias König[4] — [1]IFF, IFW Dresden, 01069 Dresden, Germany — [2]IMW, IFW Dresden, 01069 Dresden, Germany — [3]EMAT, University of Antwerp, 2020 Antwerp, Belgium — [4]IPF Dresden, 01069 Dresden, Germany

Surface plasmon polaritons (SPP) are self-sustaining resonances occurring in metallic nanoparticles. They are associated with strongly enhanced, localized electrical fields, which may be coupled to external optical excitations. SPPs can be used for the sub-wavelength control of electromagnetic fields. Based on this, novel electronic devices can be realized, for instance on-chip light spectrometers, plasmonic rectennas for the harvesting of light or LEDs and photovoltaics with a higher efficiency. SPPs can currently be mapped and hence characterized with nanometer resolution by measuring the energy-loss of a sharp electron beam in a TEM, which roughly corresponds to the z-component of the transient field. In order to record also the other components of the induced electric field, we developed a novel technique. We measure the deflection angles of inelastically scattered electrons. There, we take advantage of the fact that the measured deflection angle is proportional to the induced field components. By measuring the complete transient electric field, we comprehensively study the properties of the SPPs including associated dielectric susceptibilities and the field enhancement effect.

MM 27.2 Tue 18:30 Poster E

Contacts Between Cu and Sn Nanowires — •Zezhao Chen, Ziyi Wang, Samuel Griffiths, and Guido Schmitz — Institute of Materials Science Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany

Due to the commercial push for the size reduction of electronics and components therein, nanowires play an important role in the electronics industry. In this work, Cu-Sn nanowires have been studied, which are of scientific interest as solder-able nanostructures. The nanowires have been produced via electrodeposition using polycarbonate membranes as templates. First, Cu nanowires (50 nm in diameter) are partially grown from a CuSO4 solution and subsequently Sn is electrodeposited onto the Cu using a SnSO4 solution, resulting in segmented Cu-Sn nanowires. Furthermore, heat treatments at temperatures ranging from 220 °C - 400 °C are performed to investigate the formation of intermetallic phases within the dimensionally restricting nanowires. TEM, SEM, and EDX data has been evaluated to identify reaction products and growth mechanism.

MM 27.3 Tue 18:30 Poster E

Synthesis of Heterostructured Cu-Ni Nanowires — •Ziyi Wang, Tim Lehmann, Samuel Griffiths, Efi Hadjixenophontos, and Guido Schmitz — Institute of Materials Science Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany

In recent years, nanowires have been widely applied in electronic devices such as transistors and batteries due to their outstanding electrical conductivity and miniscule size. This work involves the research of phase stability of Cu-Ni nanowires, in order to determine whether heterostructured nanowires can form by annealing from the single phase solid solution. The whole work is separated into three steps. First, binary nanowires are prepared by electrodeposition using a porous membrane as a template. Second, different heat treatments are conducted at temperatures ranging from 130°C - 600°C in order to induce phase separation. Finally, SEM, TEM as well as EDX are utilized to analyze the nanowires. For a better understanding, Atom Probe Tomography (APT) is suggested for a 3D reconstruction of the nanowires.

MM 27.4 Tue 18:30 Poster E

Nucleation and Growth of Goldnanoparticles — •Felix Bourier, Tobias Redder, Christian Strelow, and Alf Mews — Universität Hamburg, Hamburg, Deutschland

Although inorganic nanocrystals are already used for large-scale technical and biomedical applications such as, biomarkers and drug delivery systems, their wet chemical production is still based on mainly empirical protocols. An understanding of nanocrystal formation exceeding the far too simplified classical models of nucleation and growth is still lacking.

Tracking the reduction of a gold precursor in toluene followed by the formation of nanoclusters, which then grow into particles should give better insights into the underlying mechanisms. This is achieved by combining experimental and simulated data with the use of a numerical aproached based on a set of rate equations.

MM 27.5 Tue 18:30 Poster E

Micro-mechanical behavior investigation of nanoporous gold: searching for the size of the structural unit — •Yijuan Wu[1], Jürgen Markmann[1,2], and Erica T Lilleodden[1,2] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Microcompression testing of nanoporous gold (NPG) was carried out in order to investigate the effect of the ratio of deformation length-scale to microstructural length-scale. By varying both the micropillar diameter and the NPG ligament diameter, a critical ratio was found above which the test structure can be considered a representative volume of material resulting in reproducible stress-strain behavior and uniform deformation. This critical ratio was found to be independent of microstructural length-scale, suggesting self-similarity between the different samples. Below this critical ratio, stochastic behavior is observed along with non-uniform deformation and failure, suggesting incomplete load-bearing units.

MM 27.6 Tue 18:30 Poster E

Towards 2D Topological Insulator Devices — •Katharina Polyudov[1], Kristina Vaklinova[1], Marko Burghard[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Spintronics requires the efficient generation, manipulation and detection of spin currents. Graphene has been demonstrated to be a high performance spin transport material, however due to its low spin orbit coupling (SOC), generation and control of the spin polarization by electrical means is difficult. Promising spin generators are the topological insulators (TIs), whose helical surface or edge states feature spin-momentum locking. One intriguing strategy is to locally decorate graphene by a 3D TI in order to create spin generator regions that could be smoothly integrated with laterally adjacent, bare graphene regions as spin transport channels. Along these lines, it is relevant that theory predicts that the interface-induced spin-orbit coupling (SOC) imparted by the 3D TI is able to increase the band gap of the 2D TI graphene. Here, we report the gate-dependent, low temperature charge transport properties of vertical heterostructures composed of graphene and a thin layer of Bi2Te2Se as 3D TI. By using different contact configurations, we explore the extent to which the presence of the Bi2Te2Se top layer modulates the magnetotransport properties of graphene, and furthermore whether signatures of charge transport through helical 1D edge channels within the graphene can be detected.

MM 27.7 Tue 18:30 Poster E

Transparent CdS@TiO2 Nanotextile Photoanode with Boosted Photoelectrocatalytic Efficiency and Stability — •Long Liu, Huaping Zhao, Rui Xu, Shipu Xu, Chenglin Zhang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Photoelectrocatalytic (PEC) splitting of water into hydrogen and oxygen by direct use of sunlight is an ideal and renewable method for the hydrogen production, which could integrate the solar energy collection and water electrolysis into a single photoelectrode. In this context, we report the exploration of transparent CdS@TiO2 nanotextile photoanode with boosted photoelectrocatalytic (PEC) efficiency and stability, by controllable coating of amorphous TiO2 ultrathin layer via atomic layer deposition (ALD) technique. with precise controlled thicknesses and compositions at an angstrom scale. It is found that the coated pinhole-free TiO2 layers with fixed thicknesses at 0.5-10 nm are effective to stabilize the CdS textile electrode with improved PEC efficiencies, which could not only reliably suppress the active photocorrosion, but also create a tunneling barrier for photogenerated holes, suggesting their promising application for efficient evolution of H2. It is verified that the introduced TiO2 nanoshells could limit the charge recombination, facilitate the charge separation, reduce the charge transfer resistance, and enhance the wettability of electrode, resulting in their significantly enhanced PEC performance.

MM 27.8 Tue 18:30 Poster E

Hydrogen interacting with titanium dioxide: ab initio study — •Mohsen Sotoudeh[1], Marian Bongers[2], Vladimir Roddatis[2], Jakub Čížek[3], Carsten Nowak[2], Martin Wenderoth[4], Peter Blöchl[1,2], and Astrid Pundt[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Department of Low-temperature Physics, Charles University in Prague, V Holešovičkách 2, 18000 Praha 8, Czech Republic — [4]IV. Physikalischen Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Electronic and structural properties of hydrogen doped rutile titanium dioxide has been investigated using first-principles calculations. We use density functional calculations with a band gap correction. We rationalize the various defects through the atomic and electronic structure as well as the thermodynamics. The goal is to explain the changes of electron energy loss spectroscopy (EELS) data obtained close to the Pd/rutile interface in different hydrogen environments. The calculations show that increasing the hydrogen partial pressure affects the interface concentration of oxygen vacancies and also the hydrogen content. A change of the electronic structure was observed depending on the defect types, their charge states, and their concentrations.

The work has been supported by the DFG through SFB 1073, projects C03 and C06 as well via the Heisenberg grant PU131/9-2.

MM 27.9 Tue 18:30 Poster E

HYDROGEN SORPTION KINETICS IN MgH2 AND TiH2 THIN FILMS — •Efi Hadjixenophontos[1], Lukas Michalek[1], Andreas Weigel[1], Michael Hirscher[2], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, (IMW) University of Stuttgart, Stuttgart, GERMANY — [2]Max Planck Institute for Intelligent Systems, Stuttgart, Germany, Stuttgart, Germany

Among metal hydride materials, Mg and its alloys show a great performance for the H-fuel based economy, however they still lack of performance. Transition metals eg.Ti seem to improve such systems.Here, we study separately the 2 systems:Ti-TiH2 and Mg-MgH2 in thin films (50-800nm) which enable us to monitor the hydride growth and determine the diff.coeff.The two metals show a different hydrogenation behaviour.The linear growth, due to the oxide passivation layer, in Ti, and the H diff. coeff. inside the oxide are quantified, as well as a reliable lower bound to the H diffusion coeff. in Ti is derived.The pressure dependence of H absorption is also quantitatively modelled.Micrographs support the fast diffusivity of H into Ti known from literature, since TiH2 is first formed closer to the substrate.In Mg, micrographs show MgH2 formed underneath the surface and a layer-like growth towards the substrate is observed.Surprisingly, a transition between linear (200°C) and parabolic growth regime (300°C) is observed.Resistivity measurements at the same conditions, are investigated to support this transition.Diff. coeff. and surface transport coeff. are determined by XRD,FIB and TEM.

MM 27.10 Tue 18:30 Poster E

Hydride formation in Mg-thin films — •Felix Maischner, Anshu Tyagi, and Astrid Pundt — Universität Göttingen, IMP

Magnesium is an interesting hydrogen storage material because of its high reversible hydrogen capacity in MgH$_2$ of up to 7,6 wt% and its high volumetric capacity of 110 kg/m^3 [1]. But a closed MgH$_2$ layer formed at the sample surface can block hydrogen uptake. Recently, it was shown that controlling the loading pressure allows efficient hydriding of Mg at 293 K [2]. This was interpreted by the related MgH$_2$ nuclei density. Further, the addition of grain boundaries improves the hydriding kinetics of Mg materials [3].

To study the nucleation and growth process in Mg thin films on a local scale, we perform STM measurements in an UHV-system between hydrogen loading steps. This surface sensitive method allows monitoring the hydride growth and morphology in the film via local height changes [4], as MgH$_2$ precipitates locally expand the lattice by about 30% in vertical film direction with respect to the α-phase Mg film [5]. 50 nm Mg films were prepared by cathode-beam sputtering on Si-substrates, covered with 10 nm Pd. The adhesion between the film and the substrate and its impact on the hydride morphology will be considered.

The work is funded by DFG via Project PU131/9-1 and PU131/10-2.

[1] M. Dornheim, et al., Scr. Mat. 56 (2007) 841, [2] H.T. Uchida, et al., Acta Mater. 85 (2015) 279 [3] M. Hamm, A. Pundt, IJHE 42 (2017) 22530, [4] K. Nörthemann, A. Pundt, Phys. Rev. B 83 (2011) 155420, [5] A.Baldi, et. al. Phys. Rev. B 81 (2010) 224203.

MM 27.11 Tue 18:30 Poster E

Hydrogen Diffusion in α-Magnesium: Further Investigations into the Influence of Grain Boundaries — •Felix Jung[1], Magnus Hamm[1], Jakub Čížek[2], and Astrid Pundt[1] — [1]Institute of Materials Physics, Georg-August-Universität Göttingen, Germany — [2]Department of Low-Temperature Physics, Charles University, Prague, Czech Republic

In this work we measure the room temperature diffusion coefficient of hydrogen in the α-magnesium-hydrogen system by using gas volumetry. To explore the dependency of the diffusion coefficient on the volume fraction of grain boundaries, the sample grain size is varied. Grain boundary (D_{GB}) diffusion conventionally differs from bulk diffusion (D_{V}). For substitutional solvents in metals, D_{GB} is several orders of magnitude higher than D_{V}, for interstitial solvents it can be either lower or higher, depending on the solvent concentration [1, 2, 3]. Bulk magnesium samples subjected to various degrees of severe plastic deformation are characterized using optical and electron microscopy. Purity and microstructure of the samples are investigated by EDX and EBSD measurements. The grain size distribution is examined by an automated analysis of backscatter SEM images. Details of this method are presented. Financial support provided by the Deutsche Forschungsgemeinschaft via the projects PU131/9-2 and PU131/10-1 is gratefully acknowledged.

[1] Kaur and Gust, Ziegler Press Stuttgart (1989)
[2] Mütschele et al., Scr. Metall. 21, 135-140 and 1101-1104 (1987)
[3] Uchida et al., Acta Mater. 85, 279-289 (2015)

MM 27.12 Tue 18:30 Poster E

Dehydrogenation of the hydrogen storage material sodium borohydride — •Maik Szafarska[1,2], Georgia Sourkouni - Argirusi[1,2], and Wolfgang Maus - Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal - Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal - Zellerfeld, Germany

In the last decade, sodium borohydride (NaBH4) has attracted attention in energy storage research, caused by its high hydrogen density of 10.6 wt.% and relatively low cost, making it a potentially better hydrogen (and energy) storage unit compared to compressed hydrogen gas tanks and liquid hydrogen. Therefore it would be an improvement for fuel cell economy and energy storage. To accomplish this, NaBH4 has to be stabilized against decomposition through reaction with water in humid atmospheres and the dehydrogenation process must be understood properly, especially regarding NaBH4 decomposition during dehydrogenation. To investigate the dehydrogenation process and the desorbed components of the material, Thermogravimetric- and Multi Gas-Analysis were performed. The experimental results show correlations between particle size of the material and the desorption rate of hydrogen. In addition, a semi permeable membrane was used to successfully stabilize the NaBH4 against decomposition and analyzed for its influence on the hydrogen desorption process.

MM 27.13 Tue 18:30 Poster E

Hydrogen induced defects in the palladium/rutile titanium dioxide model system — •Marian David Bongers[1], Mohsen Sotoudeh[3], Vladimir Roddatis[1], Carsten Nowak[1], Martin Wenderoth[2], Peter Blöchl[3], and Astrid Pundt[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]IV. Physikalischen Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany

The Pd/TiO$_2$ system is used in a range of applications where in particular the interaction with H is of interest. An insight into the basic interaction of H with the Pd/TiO$_2$ model system can yield to a fundamental understanding of the property-microstructure relations. We use in-situ environmental transmission electron microscopy (ETEM) and electron energy loss spectroscopy (EELS) on cross-sectional Pd/TiO$_2$ lamella focusing on the interface vicinity. The EELS studies show a small change of the Ti L edge signal in the 2 nm close vicinity of the interface, for H gas pressures of about 10 Pa. These changes are attributed to a shift in the density of states by about 1 eV, in the presence of H. This is supported by projector augmented wave code simulations using the local hybrid density functional PBE0r [1]. We suggest substitutional H to be the dominant H induced defect in bulk and nearby the interface. This work is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C03 as well via the Heisenberg grant PU131/9-2. [1] M. Sotoudeh, M. Bongers, et al., submitted

MM 27.14 Tue 18:30 Poster E

Investigations on degradation effects in SOFC fuel cells — •Hanna-Friederike Poggemann[1,2], René Gustus[2], Georgia Sourkouni[2], Christos Argirusis[3], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [3]School of Chemical Engineering, National Technical University of Athens, 9 Heroon Polytechniou St. Zographos Athens

Fuel cells are an important alternative to conventional processes of power generation. A fuel cell produces electrical power and heat directly from chemical energy. This avoids losses that can occur in conventional thermal and mechanical conversion processes during power generation. Nevertheless, the application of SOFCs for power generation is strongly limited by the life span and the robustness of the cells. In this regard, we investigated the degradation of SOFC fuel cells as a function of runtime and thermal as well as electrochemical strain. We used microscope and spectroscopic methods like Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray analysis (EDX) to investigate the microstructure and chemical composition of the anode and the cathode to get insight into changes in the elemental distribution and porosity of the fuel cells. In this context, we also examined the growth of the grains in the anode of the SOFC. Finally, we used Focused Ion Beam (FIB) tomography to gain further insight into the inner structure of the anode material.

MM 27.15 Tue 18:30 Poster E

Role of native oxide layer in silicon anodes for Li/S batteries — •Luca Silvi, Arne Ronneburg, Sebastian Risse, and Matthias Ballauff — EM-ISFM, Helmholtz-Zentrum Berlin, Berlin, Germany

Lithium/sulfur (Li/S) and Lithium/air systems are possible candidates for future electrochemical energy storage, due to higher gravimetric density compared to conventional Li-ion batteries. In these systems, a lithiated silicon (Si) electrode often replaces the Li metal anode, used as a Li ions reservoir. Detailed studies on lithiation and delithiation of Si anodes are of fundamental importance in understanding capacity fading effects. Silicon crystals are used with the native silicon dioxide (SiO2) layer: upon lithiation and delithiation, Li ions interact first with the SiO2, and subsequently intercalate in the Si crystal forming a Li/Si alloy. Due to the negative scattering length density of Li, neutron reflectometry is a powerful technique for investigating lithiation and delithiation of Si anodes. Two different Li/Si cells were prepared, one with and one without native oxide layer (removed using HF etching) on the Si anode. Both were measured at the reflectometer V6 at the BER II neutron source, to shade some light on the role of the SiO2 native layer formation and its (ir-)reversibility using both electrochemical (CV, EIS, charge/discharge) and in situ/operando neutron reflectometry measurements.

MM 27.16 Tue 18:30 Poster E

Microcalorimetric study of aluminum depositon/dissolution in BMIMCl/aluminium chloride ionic liquid — •junjie xu and rolf schuster — Institute of Physical Chemistry, Karlsruhe Institute of Technology, Fritz-Haber-Weg 2 76131 Karlsruhe

Ionic liquid systems, such as a mixture of 1-Butyl-3-methylimidazolium chloride (BMIMCl) and aluminium chloride, are promising electrolytes for aluminum batteries. In order to improve the performance of aluminum batteries, knowledge of thermodynamic properties of the electrochemical processes is required. In this study, we measured the Peltier heat of the aluminum deposition/dissolution reaction (about 10 kJ/mol at a molar ratio of BMIMCl to aluminium chloride of 1:1.7) with microcalorimetry. The positive Peltier heat corresponds to warming of the electrodes during the aluminum dissolution reaction. Consequences for the aluminum dissolution process in batteries will be discussed.

MM 27.17 Tue 18:30 Poster E

Computational thermodynamics: Meaningful phase diagrams without experimental input? — •Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

Ab-initio thermodynamic data sets, especially isobaric heat capacities, calculated within our new MD approach for lithium silicides [1,2] are presented. Further, a theoretical phase diagram is discussed, where the melting points are determined using a method based on the evaluation of diffusion behaviour. The key property, the so called diffusion coefficients, and the melting points themselves are compared with experimental data.

[1] Schwalbe et al., CMS, vol. 134, p. 48-57 (2017)
[2] Taubert et al., IJMR, vol. 108, no. 11, p. 942-958 (2017)

MM 27.18 Tue 18:30 Poster E

Examination of the partial electronic conductivity of mixed ionic and electronic conducting secondary particles — •Janis K. Eckhardt[1], Markus S. Friedrich[1], Simon Burkhardt[1,2], Limei Chen[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

Lithium ion batteries are widely used as power source in portable electrical applications. In particular with regard to optimization of existing applications or development of new technologies, it is necessary to understand the fundamentals of ionic and electronic transport inside the active cathode material. Most scientists are examining cathode materials by using composite electrodes which also contain additives influencing their electrochemical properties. To avoid such influences it is desirable to investigate the electrochemical properties of the pure active material. By using a specially designed electrochemical cell we performed electrochemical impedance spectroscopy and cyclic voltammetry measurements on single $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ (NCM-111) secondary particles to gather information about their partial electronic conductivity. A cell arrangement that was suppressing the ionic current as a response to an external voltage signal was realized by making use of ion blocking metal electrodes. The results imply a correlation between the total resistance and diameter of the secondary particle, which was used to estimate the electronic partial conductivity.

MM 27.19 Tue 18:30 Poster E

Hydrothermal Synthesis and Functionalization of $LiFe_xMn_{1-x}PO_4$ for Li-Ion Batteries — •Rouven Zeus[1], Elisa Thauer[1], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institut für Physik, Universität Heidelberg — [2]Centre for Advanced Materials, Universität Heidelberg

Hierarchically structured $LiFe_xMn_{1-x}PO_4$ with various doping levels $0 \leq x \leq 1$ has been synthesised hydrothermally. The material contains nanosized primary particles which are functionalised by carbon and agglomerate to microstructures. The effect of various precursors, organic additives and different synthesis conditions on the particle morphology and the hierarchical structuring is investigated. Electrochemical studies are applied in order to assess the feasibility of the resulting materials for energy storage in lithium-ion batteries.

MM 27.20 Tue 18:30 Poster E

TiO2 inverse opals as high-performance sodium-ion battery anodes — •Yang Xu, Min Zhou, Chenglin Zhang, Liying Liang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Study of sodium-ion batteries (SIBs) has been rapidly increasing due to the growing demand of renewable energy. Electrochemical behaves of Na-ions are expected to be different from those of Li-ions because of the larger size of Na-ion, given a same host material. We employed TiO2 inverse opals as a model material to demonstrate the role of the orderliness of atomic arrangement in determining the SIB performance. We revealed that the disordering at the surface benefits to increase the contribution of surface process, while the disordering in the bulk results in improved ion diffusion but degraded electron transport. We therefore achieved high rate capability of the TiO2 inverse opals by enhancing surface ion availability that is enabled by the enhanced solvent wettability, regardless of the type of electrolytes and the concentration of Na-ion in the electrolytes. Our work offers a possibility to realize high SIB performance by adjusting the surface kinetics of the electrodes through controlling the orderliness of the atomic arrangement. This possibility could be transplanted to other energy storage systems.

[1] M. Zhou, Y. Xu, Y. Lei, et al., Adv. Energy Mater. 2016, 1600448. [2] M. Zhou, Y. Xu, Y. Lei, et al., Nano Energy 2017, 31, 514.

MM 27.21 Tue 18:30 Poster E

Concept to describe grain boundary properties depending on misorientation and inclination — •Volker Mohles and Adrian A. Schratt — Interdisciplinary Centre for Advanced Materials Simulation ICAMS, Ruhr-Universität Bochum, Bochum, Germany

In order to characterize the geometry of a grain boundary (GB) in three dimensions, essentially five independent parameters are needed, for instance three angles for the grain misorientation and two for the GB inclination. In order to enable mesoscopic simulations of GB motion with the ability to cover virtually all GBs, a functional description of the GB energy must be chosen, ideally based on a database of pre-calculated energy values. While the orientations of all grains in a mesoscopic GB simulation can be chosen in a discrete manner (using fixed points in a database), it is desirable to have a continuous description of the energy dependence with respect to the GB plane orientation in order to allow unrestricted GB motion. This description must account for the specific symmetries and cusps imposed by the GB plane orientation in relation to the crystal orientations of both pertaining grains. For such a five parameter description, a concept is introduced and discussed with respect to the expected ability to utilize (interpolate) existing or newly simulated data points (e.g. energy values from molecular dynamics simulations), which are discrete in nature, in macroscopic continuous models.

MM 27.22 Tue 18:30 Poster E

Mechanical properties of deformed and undeformed model glass former — •Mehrdad Golkia[1], Gaurav Shrivastav[2], and Jürgen Horbach[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Theoretische Physik, Sekr. EW 71, Technische Universität Berlin, Germany

The mechanical properties of glasses depend strongly on the history of their production. New glass states can be obtained by melting a glass via an external shear field, followed by a stress relaxation after switching off the shear. Since the imposed shear stress cannot completely relax to zero below the glass transition temperature, one eventually obtains a deformed glass with residual stresses [1],[2]. Here, we compare the elastic properties of deformed glasses to those of undeformed ones, using molecular dynamics computer simulations of a Kob-Andersen Lennard-Jones mixture [3]. The elastic constants of deformed and undeformed glass samples are obtained from the analysis of stress fluctuations. While the bulk modulus and the Poisson ratio are not affected by the shear deformation, slight differences can be seen in the shear modulus as well as Young's modulus. We also compare deformed and undeformed glasses in terms of the vibrational density of states and the boson peak.

References: [1] M. Ballauff *et al.*, Phys. Rev. Lett. **110**, 215701 (2013) [2] I. Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, and G. Wilde, Acta Mater. **109**, 330 (2016) [3] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994)

MM 27.23 Tue 18:30 Poster E

Interatomic interaction governed structural and dynamical evolution in La-based glasses and melts — •Zheng Wang and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen,37077 Göttingen, Germany

Through systematic investigations on structural and dynamical properties of binary La-TM glass-forming alloys, the features of liquid states and the performances in the glasses are connected and found to be governed by the interatomic interactions. A relative loose packing in La-Cu systems from an observed positive excess volume could be the result of a combination of steep repulsion and anharmonic attraction of the potential. Based on the experimental determined potential features, properties of deformation units in glasses could be predicted from the dynamics of the melts, which also relate with the distinct relaxation behaviors. Our findings not only provide deeper insights into the glass-forming system property changes induced by interatomic interaction variations, but also shed light on designing desired metallic glasses from the characteristics of the melts.

MM 27.24 Tue 18:30 Poster E

Structural Study of the Metal Induced Crystallization of Silicon — •Max Stöber[2], Charaf Cherkouk[1], Slawomir Prucnal[2], Marcel Neubert[2], Claudia Funke[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg - Institut für experimentelle Physik — [2]Helmholtzzentrum Dresden Rossendorf - Institut für Ionenstrahlphysik und Materialforschung

Metal induced crystallisation (MIC) is a process of great interest for the design of powerful nanostructured materials in a sustainable way - using comparetively low energy and no wet chemistry. In this study the process was thermally activated using Si thin layers on Ni, Al and Cu substrates. Raman spectre reveal the diameter distribution of nanostructures and the changes in the phase structure. Furthermore, micro/nanostructures and dendrite growth resulting by layer intermixing were investigated using scanning electron microscopy (SEM). Depth profiling and chemical composition were performed by focused ion beam (FIB) and energy dispersive X-ray spectroscopy (EDX) technique.

MM 27.25 Tue 18:30 Poster E

Kinetic analysis of crystallization reaction within Co-Sn alloy — •Muna Khushaim[1,2], Fatimah Alahmary[2], Nessrin Kattan[1], and Ahmad Al-Joraid[1] — [1]Department of Physics, Faculty of science, Taibah University, PO Box 344, Medina, Kingdom of Saudi Arabia — [2]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

Co-Sn alloy is an important system for Sn- based anode materials of lithium ions batteries due to the different interesting intermetallic compounds nucleate and grow during crystallization reaction. Co -Sn alloys are applied in specific high-tech applications and hence study the kinetics of the crystallization reaction of this system and the dependency of the activation energy for crystallization on the temperature might provide a method to control the reaction and the synthesized products.In this study, Co: Sn alloy with ratio of approximately 1:3 were prepared by using metal flux method. The alloy was heated under a non-isothermal condition by using differential scanning calorimetry (DSC) at different heating rates. Microstructure characterizations of the samples have been done by using x-ray diffraction (XRD) and scanning electron microscopy (SEM). After observing the exothermic change during the DCS scanning, different kinetic methods were applied in order to determine the variation of the activation energy of crystallization with temperature. The effecting of the heating rate on the reaction model will be also presented.

MM 27.26 Tue 18:30 Poster E

Grain boundary morphologies in nanocrystalline $Pd_{90}Au_{10}$ go fractal: a simulation study of the growth kinetics — •Raphael Zeller[1], Christian Braun[2], Mingyan Wang[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

Although abnormal grain growth has been investigated for more than 70 years, our understanding of its underlying physics is still quite tenuous. For nanocrystalline materials, the situation is particularly unsatisfactory, as their dominant mode of coarsening appears to be abnormal. In samples of nanocrystalline $Pd_{90}Au_{10}$ produced by inert gas condensation, abnormal growth is marked by rapidly growing grains sending "tentacles" out into the surrounding matrix, quickly encircling nearby grains and then consuming them. The perimeters of the resulting grains—revealed in metallographic sections—resemble those of fractal objects, and the grain interiors contain a significant number of small-angle boundaries. Modifying a phase field-based model for grain growth, we assess the extent to which these observations are consistent with a growth process based on grain rotation. We find that fractality can be viewed as a consequence of regrouping contiguous matrix grains into larger, simply connected regions. The residual boundary roughness reflects the length scale of the initial grain size.

MM 27.27 Tue 18:30 Poster E

Deviation of Ti-Al-N composition during APT analysis of Ti0.4Al0.6N — •Tim Lehmann[1], Patrick Stender[1], Guido Schmitz[1], and Wolfgang Engelhart[2] — [1]Universität Stuttgart, Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Heisenbergstr. 3, 70569 Stuttgart — [2]Walter AG, Derendinger Str. 53, 72072 Tübingen

Atom Probe Tomography (APT) is a powerful technique that allows for a three dimensional chemical analysis of needle-shaped specimens. In order to study decomposition processes in TixAl1-xN-thin films, samples of different composition were produced by HiPIMS. Recent measurements on decomposed Ti0.4Al0.6N-thin films have shown deviations from the expected stoichiometry in the Ti- and Al-rich domains. For a better understanding, pure TiN and AlN powder particles are analyzed as calibration samples by APT. The observed nitrogen contents are compared to the compositions measured by gas extraction and ICP-OES. The obtained correction allows for a better analysis of the measured compositions by APT. The powder particles are transferred to W-supports and post-processed via annual milling using a Focused Ion beam (FIB). Ti0.4Al0.6N-films are heat treated in Ar-atmosphere followed by subsequent post processing via FIB-lift-outs and annular milling.

MM 27.28 Tue 18:30 Poster E

Vacancy concentrations in quenched aluminium alloy AA7150 measured by a new fast scanning calorimetry and interrupted quenching method — •Bin Yang and Christoph Schick — Institute of Physic, University of Rostock

Differential fast scanning calorimetry (DFSC) has been combined with a novel differential reheating method (DRM). Interrupted quenching at different temperatures followed by overcritical cooling enables both time and temperature-dependent investigations of vacancy concentrations in aluminium alloys during cooling from solution annealing at cooling rates between 300 K/s and 100,000 K/s. Furthermore, the effect of vacancy on precipitation is investigated. The method can potentially be transferred to similar systems or related solid-state phase transformation systems also beyond the particular system analysed in the present study.

MM 27.29 Tue 18:30 Poster E

Miniaturisation of reactively wetting SnPb micro-solder on Cu and Ni capillary tracks — •Samuel Griffiths, Patcharawee Jantimapornkij, and Guido Schmitz — Institute of Materials Science, Stuttgart, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. And although these industries have pushed practical advancements in solder technologies, little is understood about the flow kinetics and thermodynamic theory which predicts solder flow behavior. Quantification and analyses of the capillary flow behavior of eutectic Sn-Pb micro-solder on microstructured linear Ni and Cu conductive tracks is presented for multiple track widths. Solder-flow experiments have been conducted at 350°C in a reducing flux environment, resulting in reactive wetting. Parameters such as the equilibrium solder-flow distance, wetting/contour angles, and conductive track width are quantitatively linked. It is shown that, the relationship between the equilibrium solder-flow distance and track width behaves inversely for the Ni and Cu conductive tracks. Additionally, traditional contact angle control measurements are used to draw comparisons with the equilibrium angles of the solder fronts, which are the only dimensionally unrestricted wetting angles of the solder-flow experiments. Electron microscopic imaging and chemical analysis as well as theoretical modelling based on surface energy minimization are applied to support our conclusions.

MM 27.30 Tue 18:30 Poster E

Impact of UV light on the mechanical properties of collagen fibrils probed by Raman spectroscopy and Atomic Force Microscopy — •Marcus Schulze, Annika Stocker, Melanie Rogge, and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt

Collagen plays a decisive role in the development of substrates for tissue engineering. The controlled adjustment of its mechanical properties is essential and a potential strategy to achieve this is through physical treatment, such as UV light irradiation.

The focus of this study is to record the influence of heat and UV light on single collagen fibrils in situ. To that end, atomic force microscopy (AFM) was used for the simultaneous mapping of topography and modulus of type I collagen fibrils from rat tail tendon. The fibrils were probed in varied liquid environments (deionized water and phosphate buffered saline (PBS)) under UV light of varied wavelengths and temperatures of up to 45°C. Furthermore, structural changes in hydrated collagen films due to UV irradiation were investigated by means of Raman spectroscopy.

Our results showed that (UV/thermal) treatment performed in deionized water lowered the modulus of the collagen fibril. However, experiments performed in PBS-based solutions in combination with UV-B and UV-C light or thermal treatment of up to 45 °C showed an increase of the modulus within the first 30 to 40 minutes.

MM 27.31 Tue 18:30 Poster E

Subsurface Imaging of magnetic nanoparticles and measurement of nanomechanical properties of polymers and biological materials by bimodal atomic force microscopy. — •Lukas Stühn and Christian Dietz — Technische Universität Darmstadt, Darmstadt, Deutschland

We aim to observe the intrusion process of nanoparticles into human cells by bimodal frequency-modulated atomic force microscopy. To this end, a magnetic tip of an atomic force microscope is used to simultaneously detect the local mechanical properties of human HUVEC-cells and the subsurface locations of superparamagnetic ferritin nanoparticles.

We show that the mechanical characterization of biologic and polymeric matter is possible by the use of low-noise small cantilevers and photothermal excitation of the cantilever. To detect magnetic properties in a liquid environment, we increased the cantilever's oscillation amplitude several times using a backside coating of colloidal graphite. By embedding ferritin nanoparticles into a polymer-film, we studied the depth limits of the subsurface detection. High-resolution measurements of ferritin nanoparticles in liquids of different pH-values provided a first indication of the stability and organization of the protein shell. Moreover, we present images of human HUVEC-cells acquired by dynamic force microscopy.

MM 27.32 Tue 18:30 Poster E

Mechanical properties of 3D printed polymer-metal hybrid materials using FDM technology — Susanna Fafenrot, Nils Grimmelsmann, Martin Wortmann, and •Andrea Ehrmann — Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany

Fused deposition modeling (FDM) belongs to the 3D printing technologies. In FDM printing, a polymer is molten in the printer nozzle and placed line by line on the printing bed or the previous layer, respectively. Besides pure polymers, hybrid materials combining polymers with functional materials are also commercially available.

In a recent project, the mechanical properties of objects printed with metal-polymer blends were compared to pure poly(lactic acid) (PLA) printed elements [1]. Tensile and bending tests revealed that hybrid materials had significantly reduced mechanical properties. Unexpectedly, the tensile strengths of the 3D-printed objects were similar to those of the original filaments, indicating sufficient printing quality.

Our investigations show that while FDM printing allows for producing objects with mechanical properties similar to the original materials, metal-polymer blends cannot be used for the rapid manufacturing of objects necessitating mechanical strength.

[1] S. Fafenrot, N. Grimmelsmann, M. Wortmann and A. Ehrmann: Three-Dimensional (3D) Printing of Polymer-Metal Hybrid Materials by Fused Deposition Modeling, Materials 10, 1199 (2017)

MM 27.33 Tue 18:30 Poster E

Functional Principles of Nanostructured Particles as an Industrial Lubrication Oil Additive — •Alexander Beel, Katja Tönsing, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany

In contrast to conventional solid-state lubrication, the additivation with nanostructured particles not only facilitates the production of stable dispersions but also assures that particles will intrude quickly into the surface contact zone and create a protective layer.

In this contribution, we show by testing a dispersion including base oil, an additive package, and TiO_2-nanostructured particles in disc-disc triboexperiments that TiO_2-nanostructured particles yield a substantial friction reduction in specific material combinations. In order to clarify the mechanism of nanostructured particles as a lubricating agent, we discuss different approaches from literature, e.g. the ball-bearing effect, a surface polishing, the structural lubricity, rheological behavior, and a protective layer.

The friction reduction was observed in experiments where the lowest surface roughness was exhibited after the test procedure (polishing). As a consequence a titanium (dioxide) layer was built up on the disc surface which was detected with element-specific energy dispersive X-Ray analysis (EDX). By performing an experiment with used discs from a former TiO_2-dispersion experiment, we could conclude that the surface polishing and the titanium layer play an essential role for superior friction performance where a ball-bearing effect could be excluded

(Beel et al., 2017, Materials Today: Proceedings).

MM 27.34 Tue 18:30 Poster E

Mechanical Control of Atomic-Scale Transistors — •Florian Wertz[1], Torben Staiger[1,2], Fangqing Xie[1], Marcel Heinze[1], Philipp Schmieder[1], Christian Lutzweiler[1], and Thomas Schimmel[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein- Leopoldshafen, Germany

The atomic-scale transistors are devices that allow to open and close an electrical circuit by the controlled and reversible repositioning of just one or a few metal atoms. By means of a small electrochemical voltage in the millivolt range applied to a gate electrode, a few silver atoms are reversibly moved in and out of an atomic-scale junction, in this way reversibly closing and opening an electrical quantum point contact (QPC). The atomic-scale transistor is realized in an electrochemical cell at room temperature.

In the experiments presented here we integrated a three-point bending configuration within the cell to combine the electrochemical control (EC) with a mechanically controllable break junction (MCBJ) technique. With this EC-MCBJ technique we can perform mechanically controllable bistable quantum conductance switching of an atomic-scale transistor in an electrochemical environment. The device can be controlled both mechanically and electrochemically, and the operating modes can be combined, which expands the possibilities for controlling QPCs. Both operating modes of the QPC allow control with atomic-scale precision.