

MM 20: Poster session II

Time: Tuesday 18:30–20:00

Location: Poster C

MM 20.1 Tue 18:30 Poster C

Tuning mechanical stress by nano-structure — ●PHILIPP KLOSE^{1,2}, MAGNUS HAMM¹, STEFAN WAGNER², and ASTRID PUNDT^{1,2} — ¹Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — ²Institut für angewandte Materialien IAM-WK, Karlsruher Institut für Technologie, Engelbert-Arnold-Straße 4, 76131 Karlsruhe

When materials are adhered to rigid substrates, the sorption of light elements can lead to high mechanical in-plane stress.[1,2] Linear elastic theory predicts stresses in the range of -10 GPa, for 1 Hydrogen atom in Niobium.[1,2] These stresses can lead to changes in the material's properties. For low element concentrations, the mechanical stress increases linearly by the element content. However, reduction in the stress increase appear at and above the yield stress.[3] Final stress of about -3 GPa are commonly measured. The final stress can be tuned by decreasing the film thickness. For Nb films below 6 nm, linear and reversible stress increase is maintained to 1 H/Nb and mechanical stress of about -10 GPa is actually measured.[4] The range of linear elasticity can be increased to about 80 nm film thickness, by varying the lateral domain size.[5,6] This will be done by a coherently matched second phase. This work is financially supported by the DFG via project PU131/12-1. [1] U. Laudahn et al., JALCOM (1999), [2] S. Wagner et al., Appl. Phys. Lett. 92 (2008), [3] A. Pundt et al., Phys. Rev. B 61.15 (2000), [4] Hamm, M., et al. APL 106 (2015), [5] P. Klose et al. IJHE (2017),[6] P. Klose et al., submitted.

MM 20.2 Tue 18:30 Poster C

Residual Silver in Nanoporous Gold prepared by Alloy Corrosion — MAREIKE HAENSCH¹, MATTHIAS GRAF², ●WELJIA WANG³, ALEXEI NEFEDOV³, CHRISTOF WOELL³, and GUNTHER WITTSTOCK¹ — ¹Karl von Ossietzky University of Oldenburg, Institute of Chemistry, Oldenburg, Germany — ²Hamburg University of Technology, Institute of Optical and Electronic Materials, Hamburg, Germany — ³Karlsruhe Institute of Technology, Institute of Functional Interfaces, Eggenstein-Leopoldshafen, Germany

Nanoporous gold (NPG), a nanoporous bulk material, finds applications in electrocatalysis, sensing and energy storage/conversion due to its large surface-to-volume ratio, good electrical conductivity, high catalytic activity and chemical/structural flexibility. Samples with homogeneous structures up to several mm in size can be obtained by dealloying a silver-gold alloy in concentrated nitric acid or by applying a potential program. However, the dealloying process is never complete. The dealloyed NPG contains a residual fraction of silver, which can affect its catalytic properties. A recent TEM study shows that the residual silver is present in silver-rich regions which are remnants of the parent alloy. The depth distribution of these regions is still under debate. XPS with variation of the excitation photon energy was used to identify depth-dependent distribution of residual silver. NPG samples which underwent different treatments were investigated. For all samples the silver enrichment was found at the surface, which is in agreement with previous studies.

MM 20.3 Tue 18:30 Poster C

synthesis and optical characterization of plasmonic nanoparticles — ●RICARDO BAEZ^{1,2}, PAULRAJ MANIDURAI², SHIRLY ESPINOZA³, and CHARUSHEELA RAMANAN¹ — ¹Max Planck Institute for Polymer Research; Department -Molecular Electronics, Ultrafast Spectroscopy for Optoelectronics, Ackermannweg 10, 55128 Mainz, Germany. — ²Department of Physics, Faculty of Physical and Mathematical sciences, PO box-160-C, University of Concepcion, Concepcion, Chile. — ³ELI Beamlines, Institute of Physics, Czech Academy of Science, Na Slovance 2, 18221 Prague, Czechia.

Gold nanoparticles have promising potential for photonic applications due to high chemical stability and strong optical cross-sections [1,2]. These colloidal nanoparticles present a stable localized plasmon resonance (LPR), which leads to an enhancement of scattering processes of up to 1015 orders of magnitude [4]. In the present work we carried out a synthesis of gold nanoparticles (AuNPs) via a microwave-assisted technique using natural Vitamin C as the reducing agent [5]. Only water, Vitamin C and the gold salt precursor are necessary to generate the AuNPs under the influence of microwaves [6]. Previous results have shown the possibility of controlling the shape/size of colloids using

variations in radiation time. TEM micrographs reveal stable triangular, spherical, and pentagonal morphologies, with varying distribution and size [7]. The optical properties have been studied by using absorption and fluorescence spectroscopy [8,9]. Theoretical calculations have been by using boundary element method (BEM) [10].

MM 20.4 Tue 18:30 Poster C

Improving the stability of Silver Nanowires for electrodes via surface modification — ●VIOLETTA KALANCHA¹, IEVGEN LEVCHUK¹, NADINE SCHRENKER², ERDMANN SPIECKER², CHRISTOPH J. BRABEC¹, and KAREN FORBERICH¹ — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials for Electronics and Energy Technology (i-MEET), Martensstrasse 7, 91058 Erlangen, Germany — ²Institute of Micro- and Nanostructure Research and Center for Nanoanalysis and Electron Microscopy (CENEM), Cauerstr. 6a, 91058 Erlangen, Germany

The future electronic devices will be soft, flexible and even stretchable to be more human friendly in the form of wearable computers and gadgets. Transparent conductors are currently made from a sputtered film of indium tin oxide (ITO) due to its high transmittance (95% in this context), we are planning to develop a highly reproducible method of homogeneous silver nanowire synthesis with further surface functionalization by ligand exchange of organic ligands to inorganic ligands. We believe that this ligand exchange of original NWs surface ligands (PVP) can provide better interwire charge transport as well as material stability. Next, this modified Ag NWs will be investigated both in film and solution. The recent progress consists of a modified polyol synthesis resulting in Ag NWs with average diameters of 30 nm and length up to 50 μ m. High-performance transparent electrodes require thin diameter and high aspect ratio as two key structural traits that determine their film performance. References: 1.*Ye et al., Adv. Mater. 2014, 26, 6670. 2.*Li et al., Nano Lett. 2015, 15, 6722*6726

MM 20.5 Tue 18:30 Poster C

Tailoring microstructure of Ni-Mn-Ga single crystals through thermo-magneto-mechanical treatment — ●JONAS HEIDER^{1,2}, EMMANOUEL PAGOUNIS², ROBERT CHULIST³, MARKUS LAUFENBERG², and MIKHAIL FONIN¹ — ¹Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — ²ETO MAGNETIC GmbH, Hardtring 8, 78333 Stockach, Germany — ³Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland

Magnetic shape memory alloys (MSMA) are a promising type of smart material for application in actuators, sensors and energy harvesting devices due to their giant and fast strain induced by a moderate magnetic field or external stress. This strain is based on the motion of twin boundaries of adjoining martensitic twin variants with different orientations. A wide range of materials with varying modulations have been discovered exhibiting magnetic-field-induced strain (MFIS). Among those the Ni-Mn-Ga composition is the most promising MSMA with up to 7.1% MFIS in the five-layered (10M) modulated martensitic phase.

In our work we address the complex microstructure of adjoining twins in Ni-Mn-Ga single crystals in order to understand how different types of twin boundaries can be prepared, preserved and utilized for applications. Crystallographic analysis considering a monoclinic unit cell is performed to identify fine laminates between the macro-twinning planes denoted a/b-laminates. The evolution of the structure and magnetic properties is investigated depending on the thermo-magneto-mechanical treatment of single crystalline samples.

MM 20.6 Tue 18:30 Poster C

photothermal study of RGO-Ag nanowire composite in solid state — ●NISHAINA SAHADEV and AJI ANAPPARA — dept. of physics, nit calicut, nit campus p.o, calicut, india

Reduced Graphene Oxide (RGO) have been shown to exhibit excellent light-to-heat transduction owing to its broad-band absorptance (IR-to-UV range of frequencies) and negligible photoluminescence. Similarly silver nanowires also exhibit good photothermal activity. Here, we report a comparative study of the photothermal activity of RGO and its composites with Ag nanowires in solid state. While Ag nanowires has its characteristic plasmon absorption peaks at \sim 377 and 351 nm, RGO exhibits an absorption peak maxima at \sim 272 nm in the UV

range corresponding to the M-point in its electronic band structure. A photo-DSC setup with a UV-visible light source (250-450 nm) was used for carrying out isothermal photocalorimetric measurements on the samples at ~ 25 °C. Upon irradiation, the samples RGO, S1 and S2 (S1 and S2 are composites of RGO and Ag nanowires; with different mass percentages of Ag nanowire) in powder form were found to generate considerable amount of heat. An interesting observation was that the mass-normalized heat output of the composites (S1 and S2) upon light irradiation was higher as compared to RGO possibly resulting from the better light absorption in the composites as compared to RGO alone.

MM 20.7 Tue 18:30 Poster C
determination of the miscibility gap of Pt-Pd using Atom Probe Tomography — ●Yoonhee Lee and Guido Schmitz — Heisenberstr. 3, 70569 Stuttgart

Understanding the thermodynamics of alloy system is fundamental and a prerequisite to interpret the properties of the materials. So, no surprise that of most binary metallic system the phase diagrams were already well evaluated. Nevertheless, in some cases required data are missing, which holds especially for miscibility gaps at low temperature. A miscibility gap is suggested for Pt-Pd, an important alloy system essential for catalysis. Even though there were many efforts to prove the miscibility gap since Raub [1] have first claimed it with a critical temperature of approximately 770°C, still the gap remains as a dashed unclear line in the published phase diagrams [2].

In this work, we try to overcome the lack of information by applying Atom Probe Tomography (APT) to thin film structures needing only short diffusion length to establish equilibrium. APT is a cutting-edge technology, which can achieve an outstanding three-dimensional spatial resolution. Thus, it enables the study of atomic diffusion on a (sub-)nanometer length scale. Pt and Pd multilayers are deposited via ion beam sputtering and annealed at different temperatures to approach equilibrium. Then, needle-shaped samples are prepared by FIB lift-out and measured in APT. The experimentally determined miscibility gap is presented in comparison to literature data.

[1] *E. Raub, Journal of the Less-Common Metals, vol. 1, pp. 3-18, 1959. [2] *T. Massalski, Binary Alloy Phase Diagrams, 1990.

MM 20.8 Tue 18:30 Poster C
The Impact of an Effective Triple-line Energy on Solder Reflow and Difficulties in its Quantification — ●Samuel Griffiths and Guido Schmitz — Institute for Materials Science, Stuttgart University, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. Although these industries have driven vast practical advancements in solder technologies, little is understood about the impact of miniaturization on the reflow behaviour of solder on metal conductive tracks.

This work investigates the reflow behavior of Sn-based micro-solder on micro-structured Cu and Ni capillary tracks for various track widths. The results are compared both with the ideal wetting model of surface and interface energy equilibrium and a modified model containing a term for an effective triple-line energy which causes the steady state contact angles to deviate from the ideal case. Difficulties surrounding sample production, measurement and analysis are discussed. The difference between general surface roughness and substrate defect sites is discussed in relation to the quantification of an effective triple-line energy. The presence of an effective triple-line energy is confirmed through comparisons between surface energy optimisation modelling and experimental results.

Future work will entail further minimisation of sample dimensions towards a strip width of 1 micrometer and the process to achieve this as well as the inherent difficulties will be discussed.

MM 20.9 Tue 18:30 Poster C
Formation and electronic structure of tetracarboxylates under extreme conditions — ●Christian Albers¹, Georg Spiekermann², Robin Sakrowski¹, Christian Sternemann¹, Max Wilke², and Metin Tolan¹ — ¹Fakultät Physik/DELTA, TU Dortmund — ²Institut für Erd- und Umweltwissenschaften, Universität Potsdam

Iron-bearing carbonates are candidates for carbon storage in the deep Earth, therefore their physical properties and chemistry at high pressure and high temperature are in focus of recent research [1]. We present a setup to establish the conditions in the lower mantle (100 GPa, 3000 K). The required pressure is accomplished by dia-

mond anvil cells [2], in which the sample is heated double-sided by a Nd:YAG-Laser. Via combined X-ray emission and X-ray Raman spectroscopy [3] the electronic structure of the synthesized compounds at high pressure and temperature can be analyzed. Furthermore, optical Raman scattering provides information about the geometric structure. The case of siderite and magnesiosiderite will be discussed.

- [1] V. Cerantola et al., Nat. Comm. 8, 15960 (2017)
 [2] S. Petigirard et al., J. Synchrotron Rad. 24, 276-282 (2017).
 [3] C. Weis et al., Scientific Reports 7, 16526 (2017)

MM 20.10 Tue 18:30 Poster C
Liquid-Infused Nanoporous Solids as Photonic Metamaterials — Kathrin Sentker¹, Mark Busch¹, Andriy V. Kityk², and Patrick Huber¹ — ¹Institute of Materials Physics, Hamburg University of Technology (Germany) — ²Department of Electrical Engineering, Czestochowa University of Technology (Poland)

Metamaterials derive their functional properties not from the properties of the base materials, but from their newly designed, often multi-scale structures, in terms of precise shape, geometry, size, orientation, and elastic properties. Such hybrid material systems can be designed by infusing liquids in porous solids. In particular nanoporous media offer the possibility to establish structures significantly smaller than visible-light wavelengths and thus to act as photonic metamaterials, where the optical properties can be fine-tuned by the filling of the pore space. Here we present Laser-optical, x-ray and neutron diffraction experiments on monolithic nanoporous silicon, silica and alumina filled with simple (n-alkanes, water) and complex liquids (polymers, liquid crystals). These experiments allow us to gain detailed insights on the liquid distribution in the nanoporous media and the phase behaviour of the confined fluids with regard to the unconfined state. By the same token the resulting soft-hard hybrid materials exhibit novel properties typical of photonics metamaterials, encompassing optical birefringence step-wise changing with temperature, switchable optical transmission and fast electro-optical activity.

MM 20.11 Tue 18:30 Poster C
In situ TEM in Liquids Using a Si₃N₄ – Graphene Hybrid Cell Design — ●Birk Fritsch¹, Andreas Hutzler¹, Michael P. M. Jank², Robert Branscheid³, Erdmann Spiecker³, and Martin März^{1,2} — ¹Electron Devices (LEB), Department of Electrical, Electronic and Communication Engineering, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Cauerstraße 6, 91058 Erlangen, Germany — ²Fraunhofer Institute for Integrated Systems and Device Technology IISB, Schottkystraße 10, 91058 Erlangen, Germany — ³Institute of Micro- and Nanostructure Research (IMN) and Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science and Engineering, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Cauerstraße 6, 91058 Erlangen, Germany

Liquid cell transmission electron microscopy (LCTEM) is a powerful technique to investigate chemical processes *in situ* on the nanoscale. Whilst commercial cell designs have the drawback that they need to be operated in a dedicated TEM holder and do not allow EDX analyses, we present an advanced design that overcomes these limitations and allows state-of-the-art *in situ* methods such as HRTEM, or EDXS.

Due to the chosen geometry, micropatterned wells in Si₃N₄ can be sealed with multi-layered graphene to bypass the shadowing effects in conventional micromachining-based liquid cells by simultaneously providing a defined cell volume. By exploiting these features, we demonstrate quantitative investigations of reaction kinetics of metal-based nanostructures and thus gain valuable insights into the underlying processes.

MM 20.12 Tue 18:30 Poster C
A new doping method for titanium oxide layers prepared by plasma electrolytic oxidation — ●Wolfram Gilbert, Mhamed El Achhab, and Klaus Schierbaum — Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Controlled doping procedures in semiconducting metal oxides are of general interest for the fabrication of mixed systems with n-type and p-type crystallites [1]. Plasma Electrolytic Oxidation (PEO) is a versatile technique to create titanium oxide gas sensing layers of different anatase/rutile ratios and microstructures [2]. To extend the technique to doped systems (e.g. p-type conducting TiO₂) we add chromium salts to the electrolyte during PEO and investigate the effect on the resulting phase composition and microstructure of the films.

For this purpose, oxide layers were formed on a 125 μm thick ti-

tanium foil under PEO conditions, using a 12.85 mol/l H₂SO₄ electrolyte, which was supplemented by Cr₂(SO₄)₃. In the experiments, the Cr₂(SO₄)₃ concentration of the electrolyte, electrostatic and potentiostatic components, voltage steps and maximum current strength were changed systematically. Size and morphology of the generated layers were measured in cross-section by SEM. Chromium in the sample was detected by EDX. The crystal structure was determined by XRD and Raman spectroscopy.

[1] Y. Li *et al.*, *Sensors and Actuators B: Chemical* **83** (1-3), S. 160-163 (2002)

[2] M. El Achhab and K. Schierbaum, *J. Sens. Sens. Syst.* **5**, 273 (2016)

MM 20.13 Tue 18:30 Poster C

Porous titanium oxide produced by plasma electrolytic oxidation in DC operation mode and various electrolyte concentrations — ●BERND ENGELKAMP, MHAMED EL ACHHAB, and KLAUS SCHIERBAUM — Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Titanium oxide coatings produced by Plasma Electrolytic Oxidation (PEO) are of increasing scientific and commercial interest [1]. Prominent fields of applications are biomedical components and photocatalytic devices. Recent investigations revealed the potential for gas sensor technology [2]. The versatile character of PEO-produced coatings on titanium is due to the enormous scope of tailoring the coatings by using different process parameters. Many parameters serve as control levers, however, the most important are the electrical supply and the composition of the electrolyte. In our investigation we focus on the DC operation mode and the concentration of H₂SO₄ electrolyte [3]. We present layer thickness, porosity and phase composition (i.e. anatase and rutile ratio) of PEO-produced titanium oxide deduced from scanning electron microscopy, X-ray diffraction and Raman spectroscopy.

[1] T. W. Clyne and S. T. Troughton, *Int. Mater. Rev.* **63**, 1 (2018)

[2] M. El Achhab and K. Schierbaum, *J. Sens. Sens. Syst.* **5**, 273 (2016)

[3] B. Engelkamp *et al.*, *Metals* **8**, 386 (2018)

MM 20.14 Tue 18:30 Poster C

Structural phase transitions in palladium hydrogen thin films: Mechanical stress impact on critical temperatures — ●STEFAN WAGNER and ASTRID PUNDT — Karlsruhe Institute of Technology, Institute of Applied Materials (IAM-WK), Karlsruhe, Germany

Palladium hydrogen (PdH) thin films serve as model systems to study structural phase transitions under elastic and microstructural confinements. Mechanical stresses linked to hydrogen-absorption of thin films clamped onto hard substrates are used to tune the hydrogens chemical potential, changing the stability of the hydride phase. Stresses are superimposed by microstructural constraints, channelling stress relaxation processes in the films. In-situ measurements of chemical potential and mechanical stress enable the determination of the attractive H-H interaction energy and of the critical temperature of hydride formation. Thereby partially relaxed stresses yield sloped plateaus in the two-phase-coexistence region, that need to be considered in the systems thermodynamic description [1]. [1] S. Wagner, A. Pundt, *Int. J. Hydr. Energy* **41** (2016) 2727.

MM 20.15 Tue 18:30 Poster C

Containment free in-situ analysis of gold nanorod growth using disposable 3D-printed experimental chambers — ●TOBIAS ZECH, TILO SCHMUTZLER, and TOBIAS UNRUH — LKS, Friedrich-Alexander-Universität Erlangen-Nürnberg

Despite gold nanorods being used in various scientific fields, there still are some problems. Bad reproducibility, insufficient yield and time-consuming functionalization protocols are some of the burdens that must be overcome. More systematic in-situ analyses using scattering techniques like small angle neutron and x-ray scattering would go a long way to get further insight into the anisotropic growth of gold nanorods. However, the chemical procedure always requires a clean and metal-ion free environment, to successfully produce gold nanorods. Also, the synthesis differs to a slight degree from synthesis to synthesis, which makes it hard to compare experiments with seemingly identical synthetic parameters on separately performed experiments. Therefore, we designed a cheap, compact, expendable experimental chamber using 3D-printing. This way, we were able to skip the possibly erroneous cleaning procedure and make systematic experiments over various synthetic parameters. 3D printing also gives us the flexibility of using different techniques like UV-Vis spectroscopy in parallel, to draw even

more information out of our in-situ small angle scattering experiment. The chamber can be modified easily to include additional techniques like Raman and FTIR spectroscopy on the same sample volume in a containment free environment.

MM 20.16 Tue 18:30 Poster C

Interaction of polyamide 6 with galvanised steel and the influence of surface pretreatments — ●PHILIPP MORITZ^{1,2}, LISA WURLITZER^{1,2}, MARIA SONNENBERG^{1,2}, and WOLFGANG MAUS-FRIEDRICH^{1,2} — ¹Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — ²Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Nowadays polymer-metal composites play a key role in the automotive and aerospace industry. The use of lightweight sandwich structures, for example, could lead to lower fuel consumption and decreasing CO₂ emissions. In order to improve the mechanical properties of these composites, the physical interaction of the layers is of particular interest.

We have produced composite materials from galvanised steel and polyamide 6 to investigate the bonding in more detail. In order to improve adhesion, the steel surface was additionally coated with a SiO_x layer using plasma-enhanced chemical solution deposition (PECSD). In further experiments, the effect of plasma-treated surfaces on the adhesion was investigated.

The adhesion behaviour was characterised by T-Peel tests and the exposed interfaces were studied with electron spectroscopy and microscopy. The spectroscopic analysis indicates different chemical bonds, due to the presence of the SiO_x layer.

MM 20.17 Tue 18:30 Poster C

Measurements of mechanical properties and microstructure on thin Cu based alloys — ●CHRISTIAN AARON RIGONI, MARTIN PETERLECHNER, HARALD RÖSNER, and GERHARD WILDE — Institute of Materials Physics, University of Münster, Germany

The mechanical properties of alloys are essential to industrial applications. Tensile testing is thus an appropriate material characterization technique. In general, such devices are bonded to certain sample dimensions as thickness and length. Thus measurements of microscale foils are a challenging task. An important point in this setup is the previous sample preparation since the sample cutting and finishing has a noticeable impact on the performance of the measurement. This effect was investigated in detail using wire erosion, punching, water and laser cutting. We analyse mechanical properties of thin Cu rich sheets with a thickness down to about 40 μm and a length of about 4 mm that were measured with a miniaturized tensile testing device. The goal is to obtain the dependence of the ultimate tensile strength and creep behavior in dependence of different temperatures with respect to the microstructure. A Norton-Bayley plot is obtained from the creep data in order to access the material constants and the results were discussed.

MM 20.18 Tue 18:30 Poster C

Tailoring the Microstructure and Electrochemical Behavior of Li-Mn-O Thin Film Battery Electrodes — ●HENRY MÜLLER, YUG JOSHI, EFI HADJIXENOPHONTOS, CLAUDIA PETER, and GUIDO SCHMITZ — Institute of Materials Science, Chair for Materials Physics, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Lithium manganese oxides have received great attention for application in lithium ion battery cathodes. In this complex ternary system, several compositions can be used to reversibly intercalate lithium. They crystallize in various structures ranging from different cubic across orthorhombic to monoclinic crystal systems. We use sputter deposition to manufacture high-capacity thin film electrodes with different compositions. In electrodes with a higher oxygen content the largest fraction of the material has a monoclinic crystal structure. Electrodes containing less oxygen crystallize mostly in rock salt and spinel structure. This can be used to tune the electrochemical behavior and capacity of the material by controlling the oxygen partial pressure during deposition.

MM 20.19 Tue 18:30 Poster C

Tuning the Energetic Landscape of Mixed Dimensionality Perovskites — ●HARALDS ABOLINS and FELIX DESCHLER — Cavendish Laboratory, University of Cambridge, Cambridge, UK

Mixed dimensionality Ruddlesden-Popper perovskites have recently been shown to possess high performance in solar cells and greatly en-

hanced intrinsic stability relative to their bulk counterparts, which has proven the key challenge for the commercialization of perovskite-based photovoltaics. Nevertheless, the charge transport characteristics between the different phases in these materials have not been well understood. To elucidate the carrier dynamics in Ruddlesden-Popper perovskites a large single-phase grain system is developed and utilized to track the spatial distribution of the varying dimensionality domains in the resulting thin films and identify charge funneling routes into the lowest band-gap phases of the material, which are shown to be tunable, as needed for specific applications.

MM 20.20 Tue 18:30 Poster C

TEM investigations of microstructure and manganese-valence evaluation in $\text{Li}_x\text{Mn}_2\text{O}_4$ nanoparticles. — •FLORIAN SCHÖNEWALD, MAX BAUMUNG, VLADIMIR RODDATHS, MARCEL RISCH, and CYNTHIA A. VOLKERT — Institut für Materialphysik, Georg-August Universität, Göttingen

Controlling the oxygen evolution reaction (OER) is an important step in achieving a sustainable renewable energy future. At the moment, the process of generating molecular oxygen from water by chemical means is severely kinetically limited. $\text{Li}_x\text{Mn}_2\text{O}_4$ is studied here as a model electrocatalyst to understand the role of valence state and covalency on the electron transfer reaction.

The goal of this study is to control the OER by manipulating the manganese valence via electrochemical lithium de-/intercalation. Using TEM and STEM-EELS the structure and Mn valence of $\text{Li}_x\text{Mn}_2\text{O}_4$ -nanoparticles are investigated for different particle sizes and varying lithium content. Initial HR-TEM studies reveal no detectable changes in the particle surfaces as a result of lithiation cycles. In addition, TEM techniques are used to detect morphological changes in the active material after catalysing the oxygen evolution reaction with the aim to understand the underlying mechanisms.

MM 20.21 Tue 18:30 Poster C

Metal-insulator transition due to doping triggered localization — •MARTIN HOFFMANN¹, FLORIAN SIPEK¹, WOLFRAM HERGERT², and ARTHUR ERNST^{1,3} — ¹Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — ²Institute of Physics, Martin Luther University Halle-Wittenberg, Germany — ³Max Planck Institute of Microstructure Physics, Halle, Germany

Recent experiments found a doping induced metal-insulator transition (MIT) in $\text{CaRu}_{1-x}\text{Co}_x\text{O}_3$ at $x \approx 15\%$ [Adv. Sci. **5**, 1700978 (2018)], which was understood in terms of a simplified model as caused by Anderson localization. We are elaborating the idea of disorder induced localization using at first a tight-binding model for CaRuO_3 (CRO). The energy-level statistics of a direct diagonalized real-space clusters with randomly distributed Co impurities showed again hints pointing to localization. The latter reduces strongly the electron diffusion and, hence, causes the MIT. In order to support that model, we used also *ab initio* methods to study the electronic properties in Co doped CRO. The coherent potential approximation (CPA) within the Korringa-Kohn-Rostoker Green's function method (KKR-GF) allows the investigation of substitutional disorder. We observed strong variations in the density of states and the k -space energy landscape (Bloch spectral function) with increasing Co concentration – less s states and more d states appear at the Fermi energy. This result indicates as well the localization of electrons and a reduction of the electric current.

MM 20.22 Tue 18:30 Poster C

Electrochromism in Thin Film Lithium Ion Battery Electrodes — •YUG JOSHI, EFI HADJIXENOPHONTOS, JULIANE MÜRTER, ROBERT LAWITZKI, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Material Science, University of Stuttgart, Stuttgart, Germany

Numerous lithium-ion battery electrodes have been studied for their electrochemical cyclability, reversibility, capacity. An interesting aspect of these electrodes, which has not gained much attention, is the change of optical properties upon dis-/charging (or electrochromism). In this study, we show the optical response of some well-known battery electrodes namely lithium manganese oxide (LMO), lithium iron phosphate (LFP), lithium cobalt oxide (LCO) and lithium titanate (LTO). The primary focus of this study is on the in-situ electrochromic characterization of the mentioned electrodes. The LMO and the LTO are further characterized ex-situ to calculate the refractive indices of the materials using the Clausius-Mossotti equation. This equation gives the electronic resonance wavelengths which are closely related to the band structure of the material. A particularly clear change in the reso-

nance wavelength is observed upon de-/intercalation in LMO. For the LTO, since it is a phase-transformation based electrode, the optical constants in the dual phase region are represented as a combination of the pure phases, which yields information about the phase transformation mechanism. Finally, we consider options of utilizing these materials in optical integration based on silicon-based waveguides.

MM 20.23 Tue 18:30 Poster C

Microscopic Composition Analysis of Transparent Conductive ZnO:Al — •ERIC WEIKUM and GUIDO SCHMITZ — Chair of Material Physics, Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Transparent Conductive Oxides (TCO) are promising electrode materials for applications such as Light Emitting Devices and Photovoltaic. The state of the art TCO is Indium Tin Oxide, which suffers from its high cost. A possible alternative is Aluminum doped Zinc Oxide (ZnO:Al), which is studied in this work. The distribution of Aluminum Atoms is being studied using a Laser-Assisted Atom Probe, which allows chemical analysis on the nanometer scale. Tungsten tips are produced by Electropolishing and then developed using a Field Ion Microscope. These developed Tungsten tips are Sputter coated with Zinc Oxide, which is then Field Evaporated in a Laser-Assisted Atom Probe in order to obtain an atomic resolution of the chemical composition. The evaporation behavior of Zinc Oxide in High Electric Fields is being investigated at different doping concentrations and Laser intensities.

MM 20.24 Tue 18:30 Poster C

Template-Realized Functional Nanostructure Arrays for Electrical Energy Conversion and Storage — •HUAPING ZHAO, LONG LIU, YAOGUO FANG, and YONG LEI — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Functional nanostructures have gained wide concern in the contexts that rapid development of modern society raises huge requirements for modern and future devices. Facile realization of such nanostructures imposes a significant challenge for nanotechnology research and device applications. Template-based nanostructuring technique provides one promising approach to address this challenge owing to the superior geometrical characteristics of the templates. In particular, with perfectly-ordered porous anodic alumina membrane as template, perfectly-ordered nanostructure arrays of functional materials could be fabricated and are highly desirable for constructing high-performance energy devices. The functional nanostructure arrays with perfect periodicity stand as distinguished architectures thanks to their distinctive structural properties to tackle the primary challenges regarding the generation, transport and utilization of electrons, holes, ions or molecular species, etc. Therefore, functional nanostructure arrays have attracted intensive attention and yielded favorable electrochemical performance for energy conversion and storage.

MM 20.25 Tue 18:30 Poster C

LFP/Li3OCl/Si all solid state thin film battery — •KUN ZHANG, EFI HADJIXENOPHONTOS, YUG JOSHI, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Heisenberg Straße 3, 705969 GERMANY

Due to the high energy density and excellent flame resistance of solid state batteries, the cruising range of vehicles could possibly be improved and the danger of spontaneous combustion avoided, if all-solid-state batteries become available. In this work, it is studied to which extent Li_3OCl could be used as membrane in thin film all-solid-state batteries. Ion beam sputtering from a composite target of ($\text{Li}_2\text{CO}_3+\text{LiCl}$) give rise to smooth films of controlled thickness in the 100 nm to 500 nm range. The ionic conductivity is measured from RT up to 140 °C and the activation energy is evaluated to be equal to 0.57eV. A complete full battery is deposited by adding LFP and Si as thin film cathode and anode electrodes. The potential window and the capacity of the tri-layer system are investigated by Cyclic Voltammetry.

MM 20.26 Tue 18:30 Poster C

Ionic conductivity of LiBH_4 molten films — •EFI HADJIXENOPHONTOS, JANINA TRÜCK, and GUIDO SCHMITZ — Heisenbergstrasse 3, 70569, University of Stuttgart, Institute of Materials Science, Departement of Materials Physics, Stuttgart, Germany

The fast Li ion conductivity in LiBH_4 envisage its use as electrolyte in all solid state batteries. Whereas powders are commonly used, thin

films provide a tool for examining the Li transport and learning more about such complicated systems. In this work films of LiBH₄ are prepared by melting LiBH₄ powder and their thickness is minimized by using spin coating. The two methods demonstrate reproducible thicknesses from 18.6 *m when flattened with a spatula and 5.3-1.3 *m depending on the rotation speed during spin coating. All layers are characterized by SEM for their thickness and by EDX and XPS for their composition. Though XPS investigations confirm the identification of the light elements composing LiBH₄, EDX measurements reveal high oxygen quantities at the surface of the samples indicating the high sensitivity of the samples to air. The ionic conductivity is investigated by EIS and the change in the crystal structure is observed depending on temperature. The highest conductivity is achieved at 10-2 S/cm in the HT phase. Furthermore, the effect of different current collectors for improving the system is tested and Pt shows to improve the spin coating method.

MM 20.27 Tue 18:30 Poster C

Activation of methane and carbon dioxide by cationic tantalum clusters and their oxides under multi-collision conditions — •THERESA ZACH, NIKITA LEVIN, JOZEF LENGYEL, MARTIN TSCHURL, and UELI HEIZ — Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

The conversion of methane and carbon dioxide, potent greenhouse gases, to value-added products is considered as one of the most desirable reactions in chemistry. Tantalum-based clusters exhibit promising properties on the activation of methane and carbon dioxide. The goal of our experiment is to investigate the complex reaction mechanisms using kinetic modeling in different size regimes, from the bare atom to clusters containing tens of atoms. Both reactions are measured experimentally in the gas-phase by ion trap mass spectrometry under multi-collisional conditions, which allow us to study the kinetics of the reactions as a function of temperature, which is essential to determine the corresponding activation energies. Using this setup for clusters of different sizes and oxidation states, we have surprisingly observed very promising catalytic activity of $[Ta_8O_2]^+$ in reaction with CH_4 . The results suggest that the initial dehydrogenation of CH_4 to form $[Ta_8O_2CH_2]^+$ is in consecutive reaction with additional CH_4 yielding $[Ta_8O_2C_2H_6]^+$. $Ta_8O_2^+$ is then regenerated via release of the ethane. Further we intend to investigate the reactivity of Ta_n^+ clusters towards CO_2 . The preliminary results of these experiments will be presented at the conference.

MM 20.28 Tue 18:30 Poster C

Tayloring morphology and carbon functionalization of LiFe_xMn_{1-x}PO₄ — •LENNART SINGER¹, ROUVEN ZEUS¹, ENZO MORETTI¹, ELISA THAUER¹, PETER KLAR², SIMON BURKHARDT², LIMEI CHEN², MICHAEL BINNEFELD³, and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute of Physics, Heidelberg University — ²I.Institute of Physics, Justus-Liebig-University Gießen — ³Institute of Pharmacy and Molecular Biotechnology, Heidelberg University

We report on the systematic variation of morphology, agglomeration and carbon functionalization in LiFe_xMn_{1-x}PO₄ with various doping levels x and its effect on the electrochemical performance of the materials. A top-down approach applying a combination of solid-state synthesis and different post-treatment procedures such as ball milling, thermal treatment, and optical floating-zone purification is utilized to obtain pure materials with different primary particles size. Various mechanical and chemical approaches to obtain appropriate carbon coating of the active material have been used. In addition, we also report a bottom-up microwave-assisted hydrothermal synthesis route where key parameters such as precursor concentration, additives, and pH-value of the reactant were varied to obtain materials of different size and agglomeration state.

MM 20.29 Tue 18:30 Poster C

ACuFe₂(VO₄)₃ (A = Li,Na) as cathode material for lithium-ion batteries — •PATRICK SCHILLING¹, YUQUAN WU¹, ELISA THAUER¹, ALEXANDER VASILIEV², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute of Physics, Heidelberg University, Germany — ²Lomonosov Moscow State University, Moscow, Russia

ACuFe₂(VO₄)₃ (A = Li,Na) are novel mixed-spin chain materials which feasibility for application in lithium- and sodium-ion batteries has been scarcely studied. Due to multiple transition metal ions (i.e., Cu²⁺, Fe³⁺, V⁵⁺) providing potential redox centers, both materials are promising candidates for cathode materials in batteries. We report

electrochemical studies vs. Na and Li, respectively. While no significant activity in a Na-battery is found for A = Na, LiCuFe₂(VO₄)₃ shows a clear redox pair centered at 2.5 V and several weaker features which we associate with V⁵⁺/V⁴⁺ and V⁴⁺/V³⁺. Galvanostatic cycling shows continuous capacity decay from 270 mAhg⁻¹ in cycle 2 to 180 mAhg⁻¹ in cycle 10. XRD of electrodes at various stages of charging suggests the possible reversible formation of LiFeO₂ during lithium intercalation.

MM 20.30 Tue 18:30 Poster C

Water Adsorption on CuO_x and NiO_x clusters Attached to the Anatase TiO₂(101) Surface by DFT Calculations — •LEILA KALANTARI, JASMIN S. SCHUBERT, ALEXEY CHEREVAN, DOMINIK EDER, and PETER BLAHA — Institute of Materials Chemistry, Vienna University of Technology. Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

Experimental studies have shown the possible production of hydrogen through photocatalytic water splitting using metal oxides (CuO_x and NiO_x) attached on anatase TiO₂ nanoparticles. In this work, we performed density functional theory calculation to provide a detailed description of geometry, electronic properties, catalytic site and adsorption of water on Ni_nO_n ($n = 0 - 6$) and Cu_mO_n ($m = 1 - 6, n = 0 - 3$) attached to the anatase TiO₂(101) surface. The adsorption of Ni_nO_n and Cu_mO_n clusters on the TiO₂(101) surface has been studied using PBEsol exchange correlation functional with and without Hubbard correction (U). Various geometries of Ni_nO_n and Cu_mO_n have been investigated. It is found that the adsorption of a Ni atom on anatase TiO₂(101) surface is stronger than of Cu atom. Energetically, the NiO cluster prefers the bridge site oxygen atoms with an adsorption energy of 7.09 eV. We found that the Ni_nO_n and Cu_mO_n cluster adsorption energy remains about constant with cluster size which makes the formation of bigger cluster plausible as confirmed by TEM images. Water adsorbs non-dissociatively on the anatase (101) surface with an adsorption energy of 660 meV while water molecules dissociate on Cu₂O and metallic Cu attached to the anatase TiO₂(101) surface.

MM 20.31 Tue 18:30 Poster C

Enhancing photocatalytic efficiency of substoichiometric TiO_x at visible wavelengths using nano-resonators with anapole modes — •LUDWIG HÜTTENHOFER¹, FELIX ECKMANN², JAVIER CAMBIASSO³, EVANGELINA PENZA³, YI LI¹, EMILIANO CORTES^{1,3}, IAN D. SHARP², and STEFAN A. MAIER^{1,3} — ¹Nanoinstitut Ludwig-Maximilians-Universität, Königinstraße 10, 80539 München, Germany — ²Walter-Schottky-Institut Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — ³Centre for Plasmonics and Metamaterials Imperial College, 180 Queen's Gate, SW7 2AZ London, United Kingdom

TiO₂ has been shown to be a good candidate as photocatalyst also allowing for water splitting. On the other hand the semiconductors band gap only harvests the small UV portion of the solar spectrum. To permanently turn the material absorptive in the visible spectral range the material is annealed at vacuum. This induces oxygen vacancies in the TiO₂ giving rise to sub-bandgap states (OV-TiO₂). In this work we shape OV-TiO₂ into nano-disks exhibiting anapole resonances. This mode is characterized by a minimum in its far-field scattering and a maximum of electric energy inside the resonator. The goal of this work is to show that by varying the nano-disk geometry we can spectrally locate the anapole resonance within the oxygen vacancy states and therefore maximize the absorption. As a proof of concept study we want to demonstrate the exploitation of anapole modes by the preferred reduction of Ag on the resonator disks surface under 532nm laser excitation on a single particle level.

MM 20.32 Tue 18:30 Poster C

Thermal conduction in epitaxial LaMnO₃/SrMnO₃ superlattices — •DANIEL METTERNICH¹, DENNIS MEYER¹, ROLAND POTTHAST¹, JAN-PHILLIP BANGE¹, MARIUS KEUNECKE¹, VLADIMIR RODDASIS², VASILY MOSHNYAGA¹, and HENNING ULRICH¹ — ¹Physikalisches Institut, Georg-August Universität Göttingen, Germany — ²Institut für Materialphysik, Georg-August Universität Göttingen, Germany

We report on our experimental investigations of the thermal conduction in LaMnO₃ (LMO) / SrMnO₃ (SMO) epitaxial superlattice structures, grown by metal-organic aerosol deposition (MAD).

The thermal conductivity of our samples is measured with a transient thermoreflectivity setup - a method that uses a pulsed laser to heat the sample whilst a continuous wave laser measures the surface

reflectivity (TTR), and thereby the surface temperature in the time domain. We show that TTR is optimally suited for our oxide samples, which feature rather slow thermal dynamics. We elucidate the influence of different periodicities and arrangements of the layers of the superlattice. Furthermore, the thermal conductivity of the superlattice structures are compared to homogeneous LSMO, LMO, and SMO films. This in particular enables us to study the effect of the interfaces between LMO and SMO. Given the high structural quality of our superlattice, we also briefly discuss our plans to compare our findings with theoretical modelling and ultimately with first-principles calculations of phonon band structures. We acknowledge financial support by the DFG within SFB1073.

MM 20.33 Tue 18:30 Poster C

Nanoporous gold as carrier for electrochemically assisted immobilization of redox-active enzyme using a cationic binding module — •ELISABETH HENGGE¹, EVA-MARIA STEYSKAL¹, ALEXANDER DENNIG², BERND NIDETZKY², and ROLAND WÜRSCHUM¹ — ¹Inst. of Mater. Phys., TU Graz — ²Inst. of Biotechnol. and Biochem. Eng., TU Graz

An attractive application of nanoporous metals is in the field of biocatalysis, among which an important issue is related to the immobilization of enzymes that catalyze redox reactions. Here, we combine tailor-made enzymes with a nanoporous metal electrode under electrochemical control to enable regulation of the binding mechanisms and in-situ monitoring of underlying kinetics. An AuAg master alloy was used to produce self-supporting nanoporous gold samples by dealloying [3]. The pore size was optimized for immobilization by thermal annealing. As enzyme, the cytochrome P450 BM3 [2] fused to Z_{Basic2} has been chosen. It is already known that this binding module provides the possibility for oriented and selective immobilization on non-metallic carriers [1]. The influence of the surface charge on the immobilization is studied in-situ in an electrochemical cell. Simultaneously, we determine the decrease of enzyme concentration in the electrolyte by UV/VIS spectroscopy. The biocatalytic activity of this new hybrid material was investigated by using lauric acid as a model substrate. [1] Bolivar JM, Nidetzky B, Langmuir 28 (2012) 10040. [2] Valikhani D et al. Biotechnol. Bioeng. 115 (2018) 2416. [3] Steyskal EM et al. Phys. Chem. Chem. Phys. 19 (2017) 29880.

MM 20.34 Tue 18:30 Poster C

Optimization and characterization of rf sputtered LiCoO₂ cathodes — •MARCEL COUTURIER, FABIAN MICHEL, MARTIN BECKER, and ANGELIKA POLITY — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

LiCoO₂ (LCO) thin films have been grown by rf-magnetron sputter-deposition on platinum-coated Al₂O₃ (c-sapphire) substrates. Deposition parameters such as substrate temperature and the partial pressure ratio between O₂ and Ar were varied in order to find suitable parameters for a cathode offering reversible intercalation and deintercalation of lithium ions. Structural characterization was carried out using X-ray diffraction and Raman spectroscopy, revealing that the orientation as well as the crystallinity of the deposited LiCoO₂ films can be influenced by varying the O₂/Ar-ratio and simultaneously applying a sufficient substrate temperature during deposition. Furthermore, both

the atomic composition and the atomic distribution were determined using X-ray photoelectron spectroscopy and secondary ion mass spectrometry. Results showed that the films are nearly stoichiometric and have a homogeneous atomic distribution throughout the entire depth profile. For electrochemical characterization, LiCoO₂ thin films were charged and discharged against lithium metal while using a liquid electrolyte consisting of LiPF₆ dissolved in a mixture of EC/DMC with a molar fraction of 1:1. Reversible discharge capacities in the order of up to 70 mAh/g could be achieved for optimized LiCoO₂ thin films.

MM 20.35 Tue 18:30 Poster C

Development of a Neural Network Potential for Metal-organic Frameworks — •MARIUS HERBOLD, MARCO ECKHOFF, and JÖRG BEHLER — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are porous crystalline materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. To date, computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields, which in most cases are unable to describe the making and breaking of bonds. Electronic structure methods like density-functional theory (DFT) in principle offer a solution for this problem, but often the required systems are too large for routine applications of DFT. Here we present a high-dimensional neural network potential for a series of MOFs, which combines the accuracy of first principles with the efficiency of simple empirical potentials. We demonstrate that it is possible to obtain a reliable description of the potential-energy surface based on reference calculations of molecular fragments only.

MM 20.36 Tue 18:30 Poster C

In Situ Impedance Analysis of LSC Thin Films during Growth on YSZ and LSGM — •MATTHÄUS SIEBENHOFER, GHISLAIN M. RUPP, JÜRGEN FLEIG, and MARKUS KUBICEK — Institute of Chemical Technologies and Analytics, Vienna University of Technology

The mixed conducting perovskite material La_{0.6}Sr_{0.4}CoO_{3-δ} (LSC) is a very promising cathode material for application in a solid oxide fuel cell (SOFC) due to its catalytic properties for the oxygen surface exchange and its high electronic conductivity. A factor which is essential to consider in the characterization of LSC is the influence of lattice strain on the surface exchange resistance and the chemical capacitance. Recent findings showed that tensile strained films exhibit faster surface exchange and diffusion compared to compressively strained films.

In this study the influence of the two different substrates Y₂O₃:ZrO₂ and (La,Sr)(Ga,Mg)O₃ on LSC thin films was examined with a novel method allowing in situ impedance spectroscopy during the PLD process (IPLD). That way, it is possible to track charge carrier densities during growth and to link the results with microstructure and strain.

According to the measurements, tensile strain leads to an increase of the chemical capacitance by a factor of 1.6 and therefore to an increase of the effective concentration of oxygen vacancies. Furthermore a decrease of the surface exchange resistance by 50 % was observed. These results are also in agreement with previous theoretical studies which suggest that tensile in-plane lattice strain lowers the vacancy formation energy and therefore increases the vacancy concentration.