

MM 22: Poster session I

Time: Monday 19:00–20:00

Location: P4

MM 22.1 Mon 19:00 P4

Nano-scale grain substructure as a factor determining transport properties of ceramic manganites — ●ANASTASHIA NOVOKHATSKA and GENNADIY AKIMOV — Donetsk Institute for Physics and Engineering named after A. A. Galkin of the National Academy of Sciences of Ukraine, Av. Nauky 46, Kyiv, 03680, Ukraine

We present a new method for obtaining nano-scale grain substructure in $\text{La}_{0.65}(\text{Ca},\text{Sr})_{0.35}\text{MnO}_3$ manganite ceramics sintered at 1500 °C by means of excess manganese from 10 and 20 % as well as the study of its structure and magnetoresistive properties. With results of the scanning electron microscopy research, it is shown that the presence of excess manganese allows to sinter ceramics at temperatures of up to 1500 °C while maintaining the chemical and phase composition. The ceramic samples consist of manganite grains with sizes 100 μm and Mn_3O_4 hausmannite grains. Moreover, investigations of thermally etched cleaved surfaces of ceramics grains together with X-ray diffraction data showed that manganite grains have internal layered structure with the layer size of 70-140 nm where each layer is a perfect single crystal of manganite of the stoichiometric composition. It is found that the emergence of a nano-scale substructure of grains is accompanied by the resistivity drop (two orders of the magnitude) and by reduction of the slope of its temperature dependence. Moreover, the metal-insulator transition temperature is shifted towards a lower temperature and the value of the magnetoresistivity (at the applied magnetic field of 5 kOe) increase in 2.5 times.

MM 22.2 Mon 19:00 P4

Electrochemical studies on single particles of active electrode materials for lithium-ion batteries (LIBs) — ●MARKUS SEBASTIAN FRIEDRICH¹, SIMON BURKHARDT¹, LIMEI CHEN¹, MATTHIAS THOMAS ELM^{1,2}, and PETER JENS KLAR¹ — ¹Heinrich-Buff-Ring 16, 35392 Giessen — ²Heinrich-Buff-Ring 17, 35392 Giessen

Lithium intercalating and deintercalating materials such as $\text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_{1-x-y})\text{O}_2$ (NCM) have been widely investigated. These materials are of interest for lithium-ion batteries due to their high theoretical capacity and high reversibility of the intercalation/deintercalation processes. Most of the studies were carried out on composite electrodes, which not only contain the pure NCM material, but also organic binder and conductive agents. These influence the electrochemical properties of the electrode significantly. To examine the influence of the active electrode material's structure on energy storage and energy conversion of a cell system, a deeper understanding of the intrinsic properties of single (active) particles is needed. Besides widely used microelectrode setups, we developed a technique to contact individual particles in an electrochemical cell and perform measurements like CVs and EIS techniques, to characterize the pristine NCM particles with focus on conductive properties. To prepare our samples we used photolithography for structuring a photoresist on an F_xSnO_2 (FTO) coated glass substrate, to form holes of well defined size to trap single particles of NCM.

MM 22.3 Mon 19:00 P4

Electrochemical properties of hierarchically structured C-coated $\text{LiFe}_x\text{Mn}_{1-x}\text{PO}_4$ — ●ENZO MORETTI¹, CHRISTOPH NEEF¹, ELISA THAUER¹, and RÜDIGER KLINGELER^{1,2} — ¹Kirchhoff Institut für Physik, Universität Heidelberg — ²Centre for Advanced Materials, Universität Heidelberg

High-purity $\text{LiFe}_x\text{Mn}_{1-x}\text{PO}_4$ with various doping levels $x = 0.1 - 0.5$, different carbon contents, and variable primary particles size have been synthesized by a combination of solid-state synthesis, optical floating zone treatment, and ball milling. The obtained nanosized materials were assembled to larger, i.e. micrometer-sized, hierarchically structured entities by thermal treatment and usage of different organic additives. Applicability of the resulting hierarchically structured product for cathodes in lithium-ion batteries is investigated by means of cyclic voltammetry and galvanostatic cycling. The effect of both the primary and secondary particle size and the carbon ratio is studied in particular. In parallel, the obtained doping series is used to study the evolution of antiferromagnetic order at low temperature as well as the average magnetic moment per metal ion, i.e. the mean electron configuration.

MM 22.4 Mon 19:00 P4

Design of Ti-based alloys with austenitic Ni-Ti nanoprecipitates — ●SASCHA B. MAISEL¹, WON-SEOK KO², JIALI ZHANG³, BLAZEJ GRABOWSKI¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck Institut für Eisensforschung, Düsseldorf, Germany — ²Ulsan University, Ulsan, Republic of Korea — ³Massachusetts Institute of Technology, Cambridge, USA

The properties of Ni-Ti nanoparticles differ from the properties of bulk Ni-Ti, yet they retain their characteristic shape memory effect. Austenitic Ni-Ti nanoprecipitates can be dispersed in metallic matrices and it has been speculated that this may lead to transformation-based strengthening due its intrinsic shape-memory property. Such an approach is considered promising to confer so-called “self-healing” features to alloys. Here, we present a combined experimental and theoretical study of such nanoprecipitates embedded coherently in Ti-V matrices. Using our knowledge of the Ni-Ti-V phase diagram based on a combination of density-functional theory and CALPHAD methods we were able to synthesize such alloys. Preliminary SEM investigations suggest nanoparticles of $\approx 200\text{nm}$ can form in Ni-V matrices with $\approx 45\text{at.}\%$ V. Despite this progress, making samples large enough for mechanical testing remains a challenge. Thus, we study the properties of the compound using three-dimensional atomistic simulations based on the modified embedded atom method. We determine the conditions under which the martensitic transformation of such nanoparticles is triggered, which depends on the size of the particle, the composition of the surrounding matrix, temperature and strain state of the system.

MM 22.5 Mon 19:00 P4

Improved anodisation of aluminium thin films for flexible plasmonic applications — ●MATTHIAS BÖHM¹, FABIAN PATROVSKY¹, SUSAN DERENKO¹, VERA FIEHLER¹, STEPHAN BARTH², HAGEN BARTZSCH², PETER FRACH², and LUKAS M. ENG¹ — ¹Institut für Angewandte Physik, TU Dresden, Deutschland — ²Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik Dresden (FEP), Dresden, Deutschland

The future of optics heavily relies on reliably and easy-to-fabricate plasmonic materials that allow for the manufacturing of novel and versatile products and devices. Nanorod arrays (NRA), for instance, are fabricated by anodising aluminium thin films with acidic solutions [1]. However, large scale manufacturing of such structures so far has mostly shown not to be very reliable and reproducible [2].

We present an easy-to-use protocol [3] that firstly allows for the reliable substrate-bound anodisation of aluminium thin films and subsequent pore filling of anodised alumina matrices, while secondly easily promoting the NRA integration into mechanically flexible plasmonic devices. Replacing the template with an elastic material yields a novel, flexible and mechanically stretchable plasmonic composite, which allows for reproducible spectral tunability in the visible wavelength range [4].

- [1] A. Eftekhari, "Nanostructured Materials", Wiley-VHC, (2008).
- [2] M. Es-Souni and S. Habouti, *Front. Mater.* 1, 35706, (2014).
- [3] F. Patrovsky et al., *Thin Solid Films* (2016) submitted.
- [4] M. Böhm et al., *Opt. Mater. Express* (2016) submitted.

MM 22.6 Mon 19:00 P4

Theory of Polaron Band Narrowing and Phonon Renormalization due to Quadratic Electron-Phonon Coupling — ●PABLO GARCIA RISUENO, QIANG FU, and CLAUDIA DRAXL — Humboldt Universität zu Berlin, Physics Department and IRIS Adlershof

We present a novel theory of electron-lattice interaction beyond the linear-coupling regime. Based on the solution of a Holstein-Peierls-type model for quadratic electron-phonon coupling, we derive explicit analytical expressions for the eigenvalue spectrum of the Hamiltonian, resulting in a narrowing of bands as a function of temperature. Being nonperturbative, our formalism also applies in the strong-coupling case. It provides a starting point for potential applications to real materials by supplementing it with ab initio parameters.

MM 22.7 Mon 19:00 P4

Synthesis and functionalization of $\text{Li}_2\text{MnSiO}_4$ and $\text{LiFe}_{0.1}\text{Mn}_{0.9}\text{PO}_4$ for Li-ion batteries — ●KEVIN HÄUSER¹, CHRISTOPH NEEF¹, HANS-PETER MAYER², and RÜDIGER

KLINGELER¹ — ¹Kirchhoff-Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — ²Institut für Geowissenschaften, Universität Heidelberg, D-69120 Heidelberg, Germany

Two classes of materials are studied with respect to their applicability and optimisation for usage in Li-ion batteries. For hydrothermally synthesized $\text{LiFe}_{0.1}\text{Mn}_{0.9}\text{PO}_4$, the effect of the primary particle size and of hierarchical structuring of the nanosized active materials into micrometer-sized agglomerates by usage of organic additives and post-synthesis treatment is investigated. In contrast, $\text{Li}_2\text{MnSiO}_4$ was synthesized by an all-acetate precursor sol-gel process. Various carbon additives were tested to determine the optimal way of creating an embedding carbon nanomatrix to functionalize the materials. For both classes, the materials are characterised by SEM and XRD studies. The electrochemical properties are investigated by means of galvanostatic cycling and the influence of primary particle size and carbon structuring is discussed.

MM 22.8 Mon 19:00 P4

Complex Main-Group Halide Semiconductors Related to Perovskite: Aiding the Rational Design of Photovoltaics — ●ANNA J. LEHNER¹, DOUGLAS H. FABINI², HAYDEN A. EVANS², CLAIRE-ALICE HEBERT², HENGBIN WANG^{2,3}, MICHAEL L. CHABINYC², and RAM SESHADRI² — ¹Fraunhofer IWM, Freiburg, Germany — ²MRL, UCSB, USA — ³MC-CAM, UCSB, USA

Hybrid organic-inorganic lead halide perovskites have emerged as very promising materials for optoelectronic applications. It is interesting to ask whether related compounds, ideally containing less toxic heavy metals, can also show those remarkable properties.

Here we present our comprehensive approach of preparing, structurally and spectroscopically characterizing as well as computationally modeling the electronic structures of various lead-free complex metal halides using density functional theory methods.[1] We present bismuth halides and materials with optoelectronically active organic constituents and discuss distinguishing features for these functional materials, such as a defect-tolerant electronic structure and proximal lattice instabilities. By studying the correlations of composition, crystal structure and electronic structure of these compounds we focus on deepening the understanding of complex main-group metal halides' optoelectronic performance and provide a starting point for the design of new functional materials.

[1] Lehner, A.J., Fabini, D.H., Evans, H.A., Hébert, C.A., Smock, S.R., Hu, J., Wang, H., Zwanziger, J.W., Chabinyc, M.L., Seshadri, R. *Chem. Mater.* **27** (2015) 7137–7148.

MM 22.9 Mon 19:00 P4

Melting and solidification behavior of In nanoparticles embedded in crystalline Al and amorphous AlYFe — ●MARK STRINGE, MARTIN PETERLECHNER, HARALD RÖSNER, CHRISTIAN SIMON, and GERHARD WILDE — Institut für Materialphysik, WWU Münster

A reduction of the sample dimension to the nanoscale typically causes a reduction in thermal stability due to an increasing relevance of the surface contribution to Gibbs free energy. Free standing metallic nanoparticles show a melting point depression [1] whereas coherently embedded nanoparticles show an increase in transformation temperatures.

In the present work In nanoparticles are embedded in different matrices using the melt-spinning technique. The thermal behavior of these particles is analyzed using calorimetric measurements. Structural analysis is performed via transmission electron microscopy.

Focusing on the influence of interfaces between particle and matrix, nanoparticles are embedded in both an amorphous phase showing no coherent interfaces and a crystalline matrix showing (semi-)coherent interfaces. By systematic variation of cooling rates the amount of undercooling is deduced to obtain the activation energy for crystal nucleation. Nanoparticles embedded in the amorphous phase behave more like free standing nanoparticles showing a larger undercooling than nanoparticles embedded in a crystalline phase.

[1] Buffat P, Borel J-P. *Phys Rev A* **13**, 2287 (1976)

MM 22.10 Mon 19:00 P4

Numerical studies of the nucleation kinetics associated with interfaces in fcc binary systems — ●M. AJMAL CHOUDHARY and JULIA KUNDIN — Department of Engineering Sciences, Universität Bayreuth

The phase-field crystal (PFC) technique is a widely used approach for modeling crystal growth phenomena with atomistic resolution on

mesoscopic time scales. We use a two-dimensional PFC model for a binary system based on the work of Elder et al. [*Phys. Rev. B* **75**, 064107 (2007)] to study the effect of the curved, diffuse solid-liquid interface on the interfacial energy as well as the nucleation barrier. The calculation of the interfacial energy and the nucleation barrier certainly depends on the proper definition of the solid-liquid dividing surface and the corresponding nucleus size. We define the position of the sharp interface at which the interfacial energy is to be evaluated by using the concept of equimolar dividing surface (r_e) and the minimization of the interfacial energy (r_s). The comparison of the results based on both radii shows that the difference $r_e^*r_s$ is always positive and has a limit for large cluster sizes which is comparable to the Tolman length. Furthermore, we found the real nucleation barrier for small cluster sizes, which is defined as a function of the radius r_s , and compared it with the classical nucleation theory. The simulation results also show that the extracted interfacial energy as function of both radii is independent of system size, and this dependence can be reasonably described by the nonclassical Tolman formula with a positive Tolman length.

MM 22.11 Mon 19:00 P4

DFT Modelling and Size Evolution of Precipitate Clusters — ●TOBIAS STEGMÜLLER and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86135 Augsburg

One of the key roles in the manufacturing of modern metal alloys is the understanding of precipitation processes taking place during thermal treatments and their influence on many material parameters like hardness or corrosion resistance. While a lot of these processes are qualitatively well understood their quantitative control is still covered by empirical approaches.

One approach for the theoretical modelling of precipitation is the so-called cluster dynamics, by which the temporal evolution of the size distribution of precipitates can be simulated. This model was applied successfully in literature for several times to the formation of a single phase with spherical precipitate shape.

Our aim is to extend the model to more complex systems. One first step is the adaption to non spherical precipitate shapes, which needs an energetic modelling of the configurational space of all possible shapes. To perform this task we use DFT based Monte Carlo simulations and incorporate the results into the cluster dynamics formalism.

In our contribution we will show the results of our approach for the formation of the well known plate shaped Guinier Preston zones in AlCu.

MM 22.12 Mon 19:00 P4

Transmission electron microscopic examination of the precipitation growth in aluminium 2195 — ●JOHANNES LUDERSCHMID, CHRISTIAN FELBER, and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86135 Augsburg

For aerospace applications the aluminium alloy 2195 is due to its alloying elements and microstructure one of the most interesting materials, as it shows a high strength and simultaneously a low density. Especially the formation of precipitates (T1 phase (Al_2CuLi) and θ' phase (Al_2Cu)) controls the strength of the material. The formation of precursors like solute enriched regions (Guinier-Preston Zones) at room temperature is a further ability of the aluminium alloy 2195. In this study the influence of different pre-treatment (natural aging, direct quenching) and different annealing conditions (time, temperature) after the solution annealing is studied with respect to the T1 and θ' precipitation growth. In particular the influence of natural aging is investigated, as here precursor phases are formed, which already reduce the chemical driving force for the further precipitation growth during the heat treatment. The kinetics of precipitate formation and growth were investigated using transmission electron microscopy and differential scanning calorimetry. The temperature and the time are the critical parameter for a diffusion process like the precipitate growth. For that reason these parameters were modified for the heat treatment in order to identify a difference in the growing of the precipitations.

MM 22.13 Mon 19:00 P4

Synthesis of nanostructured ZnO-based gas sensing devices — ●HANAA SESO, STEFAN OSTENDORP, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, Westfälische Wilhelms-University, Wilhelm-Klemm-Str.10, Münster, Germany

Solid state sensing devices for detecting gases and determining their composition gain increasing interest in recent years. Applications exist in many different fields as e.g. industrial emission analysis or vehicle

emission control. In the present work, the well-known chemo-resistive effect of ZnO is used. Which is found in the presence of an oxidizing or reducing gas species. In combination with a 3d nano-structuring procedure based on anodic-aluminum-oxides, a large sensor surface is obtained to enhance the sensitivity compared to a flat 2d sensor structures. ZnO nano-tubes with different diameters and wall thicknesses were prepared by atomic layer deposition within the pores of porous anodic alumina membranes (PAAMs). Gold electrodes for electrical read-out were fabricated by physical vapor deposition. The morphology of the ZnO-based CO sensors were investigated by electron microscopy and atomic force microscopy, and functionality was characterized using a custom-build test station. Structural differences were tried to correlate to the sensing response of the sensor structure under different ambient temperatures and different CO concentrations. The results are analyzed systematically to draw conclusions on the underlying physical mechanisms.

MM 22.14 Mon 19:00 P4

Perfectly-Ordered Nanostructure Arrays as Potentially Promising Building Blocks for Constructing High-Performance Devices — ●HUAPING ZHAO, RUI XU, MAX SOMMERFELD, LIYING LIANG, MIN ZHOU, YANG XU, and YONG LEI — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Nanostructure arrays of functional materials have drawn great current attentions for different device applications. Among the various techniques developed for fabricating arrayed nanostructures of functional materials, template-based nanostructuring technique with porous anodic alumina membrane as template becomes more and more attractive owing to the superior geometrical characteristics. Herein, we demonstrate the utilization of perfectly-ordered porous anodic alumina membrane as template for the preparation of perfectly-ordered nanostructure arrays of functional materials. By employing the perfectly-ordered porous anodic alumina membrane as template, the as-obtained nanostructure arrays have highly-controllable and perfectly-ordered structure features in large scale, which enable them to be of great advantage for the performance improvement of devices, especially for the energy conversion and energy storage devices, including solar water splitting cells, supercapacitors, and batteries, etc.

MM 22.15 Mon 19:00 P4

Measurement and Modelling of the Efficiency of ortho/para Catalysts for Hydrogen — ●SEBASTIAN MIRZ, FLORIAN ALTENBRAND, ROBIN GRÖSSLE, and BENNET KRASCH — Tritium Laboratory Karlsruhe (TLK), Institute for Technical Physics (ITEP), Karlsruhe Institute of Technology (KIT)

The equilibrium ratio between ortho and para hydrogen is 3:1 at room temperature, whereas para hydrogen would be the only present species at absolute zero. The conversion between these two species is suppressed with time constants of the order of thousand hours in the gas phase and ten hours in the liquid phase, but can be catalytically accelerated. The TLK develops an analysis system for the hydrogen isotopologue concentration in the liquid phase in a cryogenic distillation column, based on IR absorption spectroscopy. An ortho/para catalyst is needed for the calibration of this system, due to the influence of the ortho/para ratio on the IR spectra. Therefore, an experiment is installed for the investigation of ortho/para catalyst performance at temperatures between 77 K and 400 K, to provide the necessary data for the design of this catalyst. The unique application of a Raman spectroscopy system enables the model-free real-time monitoring of the ortho/para ratio during conversion. This allows the extraction of the catalyst efficiency and additionally the distinction between physisorption and chemisorption processes. This contribution presents results of the measurement and modelling of the catalyst performance of an iron oxide catalyst.

MM 22.16 Mon 19:00 P4

Influence of metal oxides on sulfation kinetics of sodium chloride and chlorine induced corrosion — ●SEBASTIAN PENTZ¹, DANIEL OTT¹, FERDINAND HAIDER¹, and RAGNAR WARNECKE² — ¹Univ. Augsburg, Inst. f. Physik, 86135 Augsburg — ²Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads especially in waste-to-energy-plants to massive problems. At prevalent temperatures around 500°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlo-

rides. This reaction requires an atmosphere containing SO₂, H₂O, O₂ and releases HCl/Cl₂. In this work the sulfation kinetics for different parameters, like temperature, gas stream, gas components or the influence of catalytic additives is examined. The conversion rate is strongly dependent on the transformation of SO₂ to SO₃, which is catalyzed by the presence of iron oxides like Fe₂O₃ or Fe₃O₄. Further experiments are done with Al₂O₃ which is supposed to be inert in the sulfation reaction or with CaO in order to examine whether a desulfurization process can be detected. In addition to the study of the reaction rate it is possible to characterize the metal loss of samples simultaneously. Furthermore the behaviour of chlorine during the process of the corrosion was investigated. Principles of the reaction conditions in waste-to-energy-plants, especially at the superheaters, are shown and laboratory experiments regarding the kinetics of sulfation reactions are presented.

MM 22.17 Mon 19:00 P4

Crystallization of coated nanoparticles — ●CHRISTINE WALTER¹, CHRISTIAN KLEIN¹, INDRANATH CHAKRABORTY², WOLFGANG PARAK², and CORNELIUS KRELLNER¹ — ¹Physikalisches Institut, Goethe-University, D- 60438 Frankfurt am Main, Germany — ²Department of Physics, Philipps-University of Marburg, D-35037 Marburg, Germany

Nanoparticles and nanoparticle assemblies display a range of properties that can diverge from classical observed properties in the colloidal regime [1]. Gold Nanoparticles coated with ω -functionalized alkane thiols, also called nanoions, can be crystallized in a diamond-like lattice , if their functionalized layers carry opposite surface charges [2]. This novel type of metamaterial presents a well-ordered three-dimensional assembly of crystalline nanoparticles with lattice parameters of about 20 nm. However, so far no electrical or magnetic characterizations of these nanoparticle crystals have been performed.

In this contribution, we report on the technique of nanoparticle crystallization following the recipe given in [2] and we will discuss the influence of different parameters like temperature and solvent on the size of the nanoparticle crystals and discuss first magnetic measurements on these crystallized nanoparticles.

[1] B. A. Grzybowski, *CrystEngComm* 16, 9368 (2014). [2] A.M. Kalsin et al., *Science* 312, 420 (2006).

MM 22.18 Mon 19:00 P4

The new Lithography Scanner of BL1 at DELTA — ●JENNIFER BOLLE¹, MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, GEORG JÜLICHER¹, THORSTEN WITT¹, JOACHIM SCHULZ², THOMAS BECKENBACH², PASCAL MEYER³, and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, TU-Dortmund, D-44221 Dortmund, Germany — ²microworks GmbH, Schnetzlerstr 9, 76137 Karlsruhe, Germany — ³Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

There is a great demand for increasingly smaller micromechanical components. Deep X-ray lithography is a process to produce high quality microstructures with a lateral resolution in the μm -range, high aspect ratio and low sidewall roughness [1,2]. The structures are transferred by a shadow projection to a photosensitive resist [3]. At beamline 1 of DELTA synchrotron source a new X-ray lithography scanner (Jenoptik scanner (DEX01)) provided by BESSY was implemented and commissioned. The setup was characterized using test structures, exploiting different filters, bottom doses, and thermal conditions. This way optimized exposure parameters were determined and finally structures of industrial quality standards were produced. [1] A. Risse, *Fertigungsverfahren der Mechatronik, Feinwerk- und Präzisionsgerätektechnik*, Springer, 503 (2012); [2] A. del Campo, C. Greiner, *Journal of Micromechanics and Microengineering* /17(6), R81 (2007); [3] G. Feiertag et al., *Applied Physics Letters* /71(11), 1441 (1997).

MM 22.19 Mon 19:00 P4

Morphology of lithium-ion containing block copolymer electrolytes for rechargeable lithium-ion batteries — ●YINONG ZHANG, EZZELDIN METWALLI, BERNHARD SPRINGER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Block copolymers (BC) electrolytes have been recently investigated as solid-state membranes for lithium-ion batteries. Nanostructured BC electrolyte contains both, the ionic conducting as well as the high-tensile polymer domains, enabling both, high ionic conductivity and improved mechanical stability. Since the diffusion path of the lithium-

ions only follows the percolation path of the ionic conducting domain, the morphology of the BC electrolyte is an essential parameter. Theoretical studies have recently reported that the BC electrolyte phase diagrams significantly deviate from the conventional BC phase diagrams due to electrostatic interactions between polar chains and the alkali metal-ions. The morphology of ion-containing BC electrolyte was investigated using SEM and SAXS. In the current study, morphological deviation compared with that of the conventional BC phase diagrams in consistent with the theoretical studies is experimentally proved. Conductivity measurements of the Li-salt containing BC hybrid films were examined for different morphologies using impedance spectroscopy.

MM 22.20 Mon 19:00 P4

Multiplexed sensing of small molecules with silicon nanowire field effect transistors — ●STEPHANIE KLINGHAMMER¹, TETIANA VOITSEKHIVSKA², CLEMENS KIRSCHBAUM³, LARYSA BARABAN¹, and GIANAURELIO CUNIBERTI^{1,4} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Institute of Electronic Packaging Technology, TU Dresden, 01062 Dresden, Germany — ³Department of Psychology, TU Dresden, 01062 Dresden, Germany — ⁴Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The simultaneous detection of multiple targets within a single chip on a point-of-care device is attracting great attention within bio- and nanotechnology areas for more than decade[1]. Here, we demonstrate a multiplexed, label-free and real-time detection platform for small molecules like hormones, steroids, and viruses based on silicon nanowire field effect transistors (SiNW FETs). SiNW FETs are connected to a CMOS chip enabling the simultaneous readout of up to 32 FETs [2]. We particularly focus on the sensitive and selective binding of the target cortisol by using aptamers as receptors - allowing high sensitive screenings in more physiological conditions[3]. Finally we show the working principle in form of the biochip which serves as a portable, electro-microfluidic device facilitating the versatile and reliable detection of multiple samples on only one single sensor device. (1) Patolsky, F. et al., *Nanomed.* 2006, 1 (1), 51-65.; (2) Voitsekhivska, T. et al., *IEEE*, 2014; pp 173-178.; (3) Römhildt, L. et al., *ACS Appl. Mater. Interfaces* 2013, 5 (22), 12029-12035.

MM 22.21 Mon 19:00 P4

Equilibrium shapes of large nanoparticles: Wulff-construction on the atomic scale — ●MAGNUS RAHM and PAUL ERHART — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Finding the equilibrium shape of nanoparticles is a great challenge. While the classical Wulff construction provides a solution given a set of pre-defined surface energies in the continuum limit, the predictions are unreliable for medium sized nanoparticles when edge and corner sites have a sizeable effect the total energy. On the other end, numerous efforts have been made to find the global minimum shape without restrictions to crystal lattices, yet the complexity of the resulting optimization problem limits predictions to nanoparticle sizes of a few hundred atoms or less. Here, we explore the middle ground between large nanoparticles, which can be captured using the Wulff construction and very small nanoclusters. To this end, a computational technique based on Monte Carlo sampling in the variance-constrained semigrand canonical ensemble has been developed. We apply the method to a number of transition metals and demonstrate the flattening of the energy landscape with increasing particle size and describe its transition to the Wulff construction in the continuum limit. The method is also applied to particles with icosahedral symmetry, which are shown to have a much more rugged energy landscape and thus are more likely to exhibit a discontinuous size distribution.

MM 22.22 Mon 19:00 P4

Abnormal coarsening of nanoscale microstructures goes fractal — ●CHRISTIAN BRAUN¹, JULES M. DAKE², CARL KRILL², and RAINER BIRRINGER¹ — ¹Experimental Physics, Universität des Saarlandes, Germany — ²Institute of Micro and Nanomaterials, Universität Ulm, Germany

Despite the supposed rarity implicit in its name, abnormal grain growth (AGG) appears to be a rather common mode of coarsening in nanocrystalline materials, regardless of composition or synthesis route. In inert-gas-condensed nanocrystalline Pd₉₀Au₁₀, thermally induced coarsening fulfills the criteria for AGG, but with an unusual twist: here, the subpopulation of abnormally growing grains sends offshoots

in many directions into the surrounding matrix, much like a tumor spreading into nearby tissue! The resulting irregular growth fronts manifest a fractal-like morphology instead of the smooth interfaces observed in conventional samples. We have captured this phenomenon using orientation imaging based on electron backscatter diffraction and obtained a fractal dimension of about 1.2 for the grain perimeter, which is reminiscent of percolation processes, the migration of domain walls in a random field of pinning centers or fractal lines on ranked surfaces.

MM 22.23 Mon 19:00 P4

ArF-excimer laser irradiation of gold coated float glass - formation and implantation of gold nanoparticles — ●MAXIMILIAN HEINZ¹, MANFRED DUBIEL¹, LEON AVAKYAN², ARAM BUGAEV², LUSEGEN BUGAEV², JÜRGEN IHLEMANN³, and JÖRG MEINERTZ³ — ¹Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle (Saale), Germany — ²Southern Federal University, Zorge Str. 5, 344090 Rostov-on-Don, Russia — ³Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, D-37077 Göttingen, Germany

In this study, plasmonic Au nanostructures in soda-lime-silicate float glasses have been generated by gold coating and ArF-excimer laser irradiation (193 nm) of the glass surface. The formation of Au nanoparticles could be verified by the surface plasmon resonances between 530 and 600 nm, which were obtained by optical spectroscopy. Furthermore, the implantation of these nanoparticles into the glass as a consequence of melting of the glass surface by the laser has been investigated by means of electron microscopy (SEM and TEM). Here the absorption of the glass at the laser wavelength plays an important role. The implantation of the nanoparticles into the glass is an important condition to generate corrosion resistant laser marks, for example micro patterns, which are of specific interest for applications of nanoplasmonics, nanoantennas and labeling by holograms.

MM 22.24 Mon 19:00 P4

Planarization and pattern transfer at ultra-smooth aluminium surfaces — ●JENS BAUER, FRANK FROST, and THOMAS ARNOLD — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Metal mirrors are of increasing interest for the technological progress in EUV/XUV lithography, x-ray and synchrotron optics. Recently, we have presented a direct surface figuring technology, which is based on reactive ion beam etch (RIBE) processing. The use of sub-aperture ion beams allows the deterministic machining of optical Al surfaces while preserving the surface roughness almost in its initial state. Now we apply this promising technique for an advanced customization of the Al surface topography. Two cases are distinguished: 1) Surface planarization experiments are performed applying a sacrificial resist layer. Typically, several hundred nanometres of resist allow for a geometrical levelling of disturbances within the surface micro-roughness and waviness. This smooth resist topography is then transferred into the Al surface. RIBE process optimization is performed by variation of the gas composition and ion beam machining geometry to achieve a resist/Al selectivity in the order of unity. 2) Al surfaces are structured by topography transfer of a patterned resist layer via RIBE. The proportional pattern transfer is controlled by the resist/Al selectivity. The engraving of regular ultra-shallow grid patterns into aluminium is performed by a damped proportional transfer. The processes are evaluated by AFM and WLI topography measurements. A PSD analysis allows for the quantitative assessment of topography features.

MM 22.25 Mon 19:00 P4

Modeling the electrocaloric effect in ferroelectric solid solutions — ●ANNA GRÜNEBOHM¹, TAKESHI NISHIMATSU², and RALF MEYER³ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — ²Institute for Materials Research, Tohoku University, Japan — ³Department of Mathematics and Computer Science, Laurentian University, Sudbury, Canada

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field. The ECE is promising for novel cooling devices [1]. However, in many ferroelectrics the large ECE is restricted to a narrow temperature interval. Solid solutions such as Ba_xSr_{1-x}TiO₃ are promising to tune the operation range. We discuss possible routes of modeling disordered solid solutions by means of *ab initio* based molecular dynamics simulations [2,3]. Furthermore, we present direct simulations of the ECE for Ba_xSr_{1-x}TiO₃ [4].

[1] X. Moya, *et al.*, *Nature Mater.* **13**, 439 (2014).

[2] T. Nishimatsu *et al.*, *J. Phys. Soc. Jpn.* **85**, 114714 (2016).

- [3] S. Tinte *et al.*, J. Phys.: Condens. Matt. **16**, 3495 (2004).
 [4] M. Marathe, *et al.*, Phys. Rev. B **93**, 054110 (2016).

MM 22.26 Mon 19:00 P4

Tuning of the optical properties from alloy nanoparticles with varied compositions sputtered from one target — ●WIEBKE REICHSTEIN¹, ALEXANDER VAHL¹, JULIAN STROBEL², OLEXANDR POLONSKYI¹, THOMAS STRUNSKUS¹, LORENZ KIENLE², and FRANZ FAUPEL¹ — ¹Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — ²Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Synthesis and Real Structure, Kaiserstr. 2, 24143, Kiel, Germany

Optical properties like particle plasmon polaritons of elemental noble metal nanoparticles were well studied over the past years. Recently, alloy metal nanoparticles have generated increasing interest due to their additional functionalities. In this work the optical properties of multiple stacks of silver-gold alloy nanoparticles in a transparent matrix are investigated. Nanoparticles were deposited using a Haberland type single DC magnetron gas-aggregation-source and are incorporated into a silicon dioxide matrix (pulsed reactive DC magnetron sputtering). UV-vis transmission spectra were obtained on samples where the gold concentration in the nanoparticles was varied from 60 to 75 at% leading to corresponding shifts of the plasmon resonance peak positions. Furthermore, the influence of nanoparticle agglomeration on the appearance of the plasmon absorption band was analyzed which could allow optical control of the deposition process.

MM 22.27 Mon 19:00 P4

Nano Structuring with New High-Resolution and Longtime-Stable Liquid Metal Ion (Alloy) Sources — ●TORSTEN SCHNEIDER-RAHDER^{1,2}, ACHIM NADZEYKA², LARS BRUCHHAUS², SVEN BAUERDICK², PAUL MAZAROV², MICHAEL KAHL², and ANDREAS-DIRK WIECK¹ — ¹Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — ²Raith GmbH, Dortmund

To generate structures on scales of micro- or nanometers, metal ions and clusters can be used, because their de Broglie wavelength is much smaller than that of light. This allows a higher resolution also of structures smaller than the wavelength of light. In fact, the resolution limit is more on the side of the instrumentation than due to the de Broglie wavelength, being of the order of only $\lambda = h/\sqrt{2mE} = 20$ fm (mass 70 amu, $E = 30$ keV). Metal ions emitted by liquid metal ion sources (LMIS) are bunched to a focused ion beam (FIB). Most of the commercial applications use Ga⁺ ions; here drawbacks exist due to unwanted implantation. Thus the fundamental goal of the current project is to investigate alloys consisting of different other metals, which show a eutectic behavior and are suitable to achieve a longtime-stable operation of the LM(A)IS. First, the sputtering yield of a LMAIS emitting Au⁺, Au⁺⁺ and Si⁺⁺ ions will be analyzed according to the beam current and the dwell time. For these measurements, samples of Si, Cr, Au and others will be used. Subsequently, more parameters will be varied in order to maximize the removal rate and the resolution. Similar investigations will be conducted using other alloys containing different metals (basically Bi) to optimize their operating conditions as well.

MM 22.28 Mon 19:00 P4

Ferrite filled carbon nanotubes vs. ferrite nanoparticles as anode materials for lithium ion batteries — ●LUCAS MÖLLER¹, ALEXANDER OTTMANN¹, RÜDIGER KLINGELER^{1,2}, RASHA GHUNAIM³, and SILKE HAMPEL³ — ¹Kirchhoff Institute of Physics, Heidelberg University — ²Centre for Advanced Materials, Heidelberg University — ³Leibniz Institute for Solid State and Materials Research (IFW) Dresden

Various nanosized ferrite MFe₂O₄ (M = Fe, Co, Ni) materials incorporated into multiwalled carbon nanotubes (CNT) have been studied as anode materials for Li-ion batteries. Electrochemical measurements by means of cyclic voltammetry (CV) and galvanostatic cycling with potential limitation (GCPL) were carried out in Swagelok-type two-electrode cells against Li/Li⁺. In order to evaluate the benefits of the CNT shells, the results are compared to pristine ferrite MFe₂O₄ nanoparticles. The CVs show typical redox activity associated with the conversion reaction $MFe_2O_4 + 8Li^+ + 8e^- \leftrightarrow M + 2Fe + 4Li_2O$. For the functionalised nanotubes, the data show in addition signatures of Li de-/intercalation into the CNTs. GCPL measurements reveal better cycling stability of the CNT-incorporated compared to the pristine ferrite nanoparticles.

MM 22.29 Mon 19:00 P4

Characterization of different para-quinones as electrode materials in Li-ion batteries — ●CHRISTINA SCHMIDT¹, YUQUAN WU¹, SEBASTIAN HAHN², FELIX HINKEL², and RÜDIGER KLINGELER^{1,2} — ¹Kirchhoff Institute of Physics, Heidelberg University, Germany — ²Centre for Advanced Materials, Heidelberg University, Germany

The applicability of various para-quinones as electrode materials in lithium-ion batteries has been studied by means of cyclic voltammetry and galvanostatic cycling. The aza-para-quinones under study have been synthesized by classic condensation reactions with established procedures. Particular emphasis is given to the preparation of the solid electrodes and to the influence of the electrolyte. Our data imply that up to 3 Li⁺-ions per molecule can be stored electrochemically, which, in the example of 5,7,12,14-tetraaza-6,13-pentacenequinone (TAPQ), are associated with reversible redox reactions at potentials between 1.8 and 3.0 V vs. Li/Li⁺. Except for the first few cycles which show relatively high capacities above 300 mAh/g, the electrodes suffer from strong fading effects. No significant improvement of the cycling stability is observed when using different carbon additives or an ether-based electrolyte.

MM 22.30 Mon 19:00 P4

Grain boundary and triple junction segregation: Comparison between atom probe experiments and atomistic simulations — RÜYA DURAN, DANIEL BEINKE, ●SEBASTIAN EICH, and GUIDO SCHMITZ — Institut für Materialwissenschaft, Universität Stuttgart

In nanocrystalline materials, the volume fractions of grain boundaries (GBs) and triple junctions (TJs) gain significance, justifying these defects as a major research topic. Excess solute segregation at those defects generally reduces the free energy of the system and may inhibit grain growth and lead to stabilization of nanocrystalline materials.

Atom probe tomography (APT) is a state-of-the-art technique with nanometer accuracy in order to obtain 3D information of the spatial chemical distribution, allowing conclusions about GB segregation amplitude and GB compositional width.

However, both the field evaporation process in APT experiments and the reconstruction algorithm *eo ipso* imply artifacts in the reconstructed sample, e.g. drastic differences of atomic densities in the GBs as compared to the bulk.

By comparing experimentally investigated two-component nanosized samples with realistic computer-simulated tricrystals, subjected to subsequent simulated evaporation, we reveal influences of the actual evaporation process on the reconstructed tip. Density fluctuations can directly be linked to different evaporation fields, which result from structural effects (e.g. different bonding in GBs) and/or different chemical species.

MM 22.31 Mon 19:00 P4

Viscoelastic and structural relaxation processes in Bombyx mori silk fibers studied by in situ X-ray scattering experiments — ●JAN ROSIGKEIT¹, IGOR KRASNOV¹, and MARTIN MÜLLER^{2,1} — ¹Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel — ²Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht

The mechanical properties of silk fibers are studied using an in situ combination of tensile tests with X-ray scattering experiments. We report our results about the viscoelastic relaxation. Structural relaxations in silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The phenomena can be well described by models based on fractional calculus. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional viscoelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history. The relaxation behavior could be well described with the fractional viscoelastic theory.

MM 22.32 Mon 19:00 P4

Optical characterization of thin-film electrode materials during electrochemical measurements — ●TIM THEIL, NELLY SANCHEZ, YUG JOSHI, SUSANN NOWAK, and GUIDO SCHMITZ — Institut für Materialwissenschaft, Universität Stuttgart

Thin-film battery electrodes are mainly characterized using electrochemical methods like cyclic voltammetry and chronopotentiometry. Using optical measurements additional insights into processes happen-

ing in the electrode materials or at the interfaces during cycling can be gained. Monitoring in-situ during lithiation and delithiation can give insight into chemical reactions or thickness changes. The approach is proven using lithium cobalt oxide (LCO) as an example for a cathode and lithium titanate (LTO) as an example for an anode. Both materials were prepared by ion beam sputter deposition on platinum coated silicon wafer with oxygen as reactive gas. LCO was crystallized by post annealing at 600°C whereas LTO was in situ annealed at 600°C. For the measurement a liquid cell with a three electrode setup was used where the used electrolyte was 1 molar LiClO₄ in EC:DMC, the counter and the reference electrode was pure lithium metal. During cycling the sample was illuminated in a 45° angle by a tungsten source and each second a reflectance spectrum was acquired at 90° to the incoming beam. The reversible dependence of the optical properties on the charge state of the materials can be clearly shown.

MM 22.33 Mon 19:00 P4

Electrochemical Strain Microscopy for mapping ionic conductivity with high spatial resolution — ●NINO SCHÖN^{1,2}, SVENJA BENNING^{1,2}, ROLAND SCHIERHOLZ¹, and FLORIAN HAUSEN^{1,2} — ¹Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, 52425 Jülich, Germany — ²RWTH Aachen University, Institute of Physical Chemistry, 52074 Aachen, Germany

Devices for energy storage play an important role in our daily life but also in tackling fundamental problems towards a sustainable energy landscape. Currently challenging is the ability to store surplus energy and release it on demand. All-solid-state Lithium-Ion-Batteries (ASSLiB) present an attractive solution with high potential for further development. To realize improved solid state batteries, it is of utmost importance to understand the electrochemical and charge transport properties of promising energy materials at a relevant scale, especially the correlation between microstructure and local Li-Ion conductivity.

Within this contribution we introduce Electrochemical Strain Microscopy (ESM) as a method to investigate ionic conductivities with very high spatial resolution. ESM is based on Atomic Force Microscopy, a powerful tool to get insights into the surface characteristics at the nanometer scale. The underlying principle of ESM is the link between the Li-Ion concentration and the molar volume. Ionic conductivity can be detected indirectly by applying a localized voltage pulse and inducing Li-Ion movement the resulting material strain can be quantified with subnanometer resolution. Hence, ESM allows for direct correlations between ionic conductivity and microstructure.

MM 22.34 Mon 19:00 P4

A detailed atomic investigation of the clustering and precipitation on a Friction-Stir-Welding simulated Al-Cu-Li(-Mg) alloy (AA2198) — ●DANNY PETSCHKE, FRANK LOTTER, and TORSTEN STAAB — Lehrstuhl für Chemische Technologie der Materialsynthese, Röntgenring 11, 97070 Würzburg

Al-Cu-Li(-Mg) alloys find wide applications in aviation and aerospace technology due to the reduction of weight and their high strength at the same time. After rolling sheets of these alloys, a defined heat treatment, following the solution annealing, leads to the formation of mainly T1-precipitates (Al₂CuLi). These precipitates are highly efficient in blocking dislocation movements and, therefore, are responsible for the high strength of the alloy. When these sheets are joined by Friction-Stir-Welding (FSW), temperatures occurring in the Weld-Nugget (WN) are close to the material's solution treatment temperature (490-510°C). Hence, the T1-precipitates are completely dissolved in this region, which results in a significant hardness-drop of 25%. Obviously, only GP-zones/GPB-zones and CuMg-clusters of several Ångström in size are formed directly after welding by diffusion processes not understood in detail, yet. We followed the precipitation kinetics directly after Friction-Stir-Welding with DSC, SAXS and Positron-Annihilation-Spectroscopy (PAS). Therefore, a Welding-Simulator was developed to reproduce the temperature profile in the welded material.

MM 22.35 Mon 19:00 P4

Characterization of materials for all-solid-state batteries prepared by ion-beam sputtering — ●SUSANN NOWAK¹, FABIAN WUNDE², JULIANE MÜRTER¹, GIULIO CALCAGNO¹, PRIANYKA SHARMA¹, YUG JOSHI¹, TIM THEIL¹, and GUIDO SCHMITZ¹ — ¹Heisenbergstr. 3, 70563 Stuttgart — ²Wilhelm-Klemm-Str. 10, 48149 Münster

All-solid-state batteries are discussed as a solution for the challenges lithium-ion batteries are facing in the moment. An all-solid-state bat-

tery is a complex system consisting of a cathode, an electrolyte, an anode and different current collectors. For the purpose of creating an all solid-state battery different materials for all of these components have to be prepared and characterized. This contribution presents the properties of different battery materials which were successfully produced using ion-beam sputtering. In particular, the fabrication and properties of LFP, LMO, LCO, Sn, Si and LiPON as thin films are shown. All-solid-state batteries which were prepared using these materials are shown and were characterized by temperature dependent cyclic voltammetry and TEM investigations. It is shown that the cycling stability is largely dependent on the chosen anode material, when lithium and tin are compared.

MM 22.36 Mon 19:00 P4

Understanding chemical ordering in intermetallic clathrates — ●MATTIAS ÅNGQVIST and PAUL ERHART — Department of Physics, Chalmers University of Technology, Sweden

Clathrates are periodic structures that provide a framework that can trap large, loosely bound species. Intermetallic clathrates often have low thermal lattice conductivity and high electric conductivity, which makes them interesting candidates for thermoelectric applications. These materials exhibit a great variability with respect to elemental composition and the distribution of the species, which provides flexibility for tuning properties but also poses a challenge with regard to developing a comprehensive understanding of these systems. Here, we demonstrate a method that can both accurately and efficiently sample this compositional space. We use density functional theory calculations to parametrize alloy cluster expansions (CE) to obtain *ab-initio* accuracy in Monte Carlo simulations that can exhaustively sample the compositional space. We apply this methodology to study the chemical ordering and related effects in the binary clathrates Ba₈Al_xSi_{46-x}, Ba₈Al_xGe_{46-x}, Ba₈Ga_xGe_{46-x}, and Ba₈Ga_xSi_{46-x} in terms of composition and temperature. We validate our method by predicting the site occupancy factors (SOFs) and achieve excellent agreement with experimental results. This validation enables us to provide a rationale for the extreme SOF behavior with varying Al content by looking at the actual interactions found in the CE. Finally, we address the contributions of chemical ordering on heat capacity and lattice expansion.

MM 22.37 Mon 19:00 P4

In situ functionalization and spectroelectrochemical characterization of gallium nitride surfaces for novel hybrid sensing platforms — ●PRINCIA SALVATORE, EUGEN SPEISER, and NORBERT ESSER — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Schwarzchildstr. 8, 12489 Berlin

Inspired by the existing semiconductor technology and encouraged by the unique set of optical and electronic properties of gallium nitride (GaN), the integration of such a material in novel sensing platforms has been attempted proceeding through a solution-based in situ modification of GaN surfaces via a phosphonic acid (PA) linkage. In contrast to other harsher functionalization routes, this approach offers the opportunity to prepare samples in solution with no need of removing oxide layers, and to exploit the side/end groups of PA derivatives for GaN surfaces terminating with different chemistries. PA adsorbates based on terpyridine are under investigation with the aim of exploring robust surface-confined layers for metal ions chelation and sensing in solution. A dual investigation by interfacial electrochemistry and optical spectroscopy (Raman and photoluminescence analysis), referred to as spectroelectrochemistry, serves to verify efficiency of the surface modification scheme and sensitivity of the sensing route, which applies to functionalized GaN crystals as planar or nanostructured surfaces. Under a monochromatic light excitation and bias, insight into interfacial processes (surface assembly, charge transfer, band bending, etc.) is gained towards the creation of novel hybrid sensors, based here on the highly controlled deposition of PA derivatives on GaN electrodes.

MM 22.38 Mon 19:00 P4

Investigation of molecular orientation in individual metal-organic nanowire by polarized raman spectroscopy and simulation — ●YANLONG XING¹, EUGEN SPEISER¹, DHEERAJ KUMAR SINGH², PETRA DITTRICH³, and NORBERT ESSER¹ — ¹Leibniz-Institut für Analytische Wissenschaften, ISAS e.V., 12489 Berlin, Germany — ²Department of Chemical Physics, Jacobs University, 28759 Bremen, Germany — ³Department of Biosystems Science and Engineering, ETH Zürich, 8093 Zürich, Switzerland

To study the molecular self-organization in conductive metal-organic

nanowire, single gold-tetrathiafulvalene (Au-TTF)nanowires were analysed using non-destructive polarized Raman spectroscopy at room temperature. A first investigation was done for neutral tetrathiafulvalene (TTF) crystal. Based on the density functional theory calculation of molecular Raman tensor and simulation of depolarization ratio, the orient of TTF molecules in a single TTF crystal was revealed. The high correlation between the results from this work and that of reported work proved the efficiency of the proposed method in this work. Afterwards, both the experimental and simulation method for TTF crystal was applied to study a single Au-TTF nanowire. It was indicated that there were at least two different molecule configurations in the wire, both tilted with respected to the long axis of the wire. The 3D model of sing Au-TTF wire showed a vivid image of molecular configurations in the wire. Compared to the proposed mechanism in reported work, this improved model can better explain the growth mechanism of Au-TTF wires with various morphologies.

MM 22.39 Mon 19:00 P4

Mechanical alloying of Ti-25Ta for biomedical applications: Effect of milling parameters — ●YANFEI SUI¹, MARIANA CALIN¹, SERGIO SCUDINO¹, CHUNMING ZOU², ZUNJIE WEI², and JÜRGEN ECKERT³ — ¹IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — ²National Key Laboratory for Precision Heat Processing of Metal, Harbin Institute of Technology, Harbin 150001, China — ³Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

The influence of milling parameters, such as milling time (10h-80h), milling speed (200rpm, 250rpm, 300rpm), as well as the initial powder morphology, have been investigated. The microstructure of the milled powder has been characterized by scanning electron microscopy, coupled with X-ray diffraction. The results indicate that, the interval milling mode that carried out with a speed of 250rpm, shows optimized mechanical alloying effect. At the initial stages of ball milling a significant broadening of the diffraction peaks was observed, which can be linked to phason strain of the quasilattice. With increasing milling time, the diffraction signals belonging to β phase were no longer observed, indicating a complete transformation of β phase to α phase. The milled powder can be further used to synthesize compacts with a low elastic modulus for biomedical applications.

MM 22.40 Mon 19:00 P4

Mechanical alloying of Ti-25Ta for biomedical applications: Effect of milling parameters — ●YANFEI SUI¹, SERGIO SCUDINO¹, CHUNMING ZOU², ZUNJIE WEI², MARIANA CALIN¹, and JÜRGEN

ECKERT³ — ¹IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — ²National Key Laboratory for Precision Heat Processing of Metal, Harbin Institute of Technology, Harbin 150001, China — ³Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

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MM 22.41 Mon 19:00 P4

An Improved Method for Point Deflection Measurements on Rectangular Membranes — ●BENOIT MERLE¹, KYLE NICHOLSON¹, ERIK HERBERT², and MATHIAS GÖKEN¹ — ¹Materials Science & Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU) — ²Department of Materials Science & Engineering, Michigan Technological University

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