KFM 25: Poster

Time: Thursday 15:00–18:00 Location: P2

KFM 25.1 Thu 15:00 P2

Ferroelectric properties of $(Na_{0.5}Bi_{0.5})TiO_3$-$BaTiO_3$ perovskite ceramics modified by LiF additives — •Sobhan M. Fathabad[1], Vladimir V. Shvartsman[1], Ekaterina D. Politova[2], Galina M. Kaleva[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, Essen, Germany — [2]Moscow

The system of $(Na_{0.5}Bi_{0.5})TiO_3$-$BaTiO_3$ solid solutions has attracted considerable interest due to its promising electromechanical, electrocaloric, and energy storage properties. In this work, the effect of LiF additive on the ferroelectric properties of $0.8(Na_{0.5}Bi_{0.5})TiO_3$-$0.2BaTiO_3$ ceramics is investigated. The samples were prepared by the conventional solid state synthesis technology. The LiF content varied from 0 to 15 mol

KFM 25.2 Thu 15:00 P2

Strain and defect location in the cross-section of laterally aligned SnO2 NWs — •Jasmin-Clara Bürger, Sebastian Gutsch, and Margit Zacharias — Laboratory for Nanotechnology, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

The 1D structure and the high surface-to-volume ratio of SnO2 nanowire-based devices allow for high sensitivities in gas- and biosensing. By their self-alignment towards the substrate edge and by the self-alignment of the SnO2 nanowire crystal lattice towards the atomic arrangement on the substrate surface[1], laterally aligned SnO2 NWs are superior to freestanding NWs as a basic structure for a single-NW-based sensor. However, up to now, only little is known about their crystal quality compared to the excellent material quality of freestanding NWs. Hence, here, laterally aligned SnO2 NWs on r-plane sapphire substrates were grown by the vapor-liquid-solid mechanism and morphologically analyzed by scanning electron microscopy. By focused-ion beam preparation, cross-sectional TEM lamellas of the laterally aligned SnO2 NWs on r-plane sapphire were prepared. For analysis of the NW defect density, post-processed strain maps were computed of atomically resolved TEM images. The theoretical background for the experimentally observed location of the lowest strain density close to the substrate-NW interface and the highest defect density close to the NW surface will be discussed.

[1] J.-C. Bürger et al., Cryst. Growth Des. (2021), 21 (1), 191-199

KFM 25.3 Thu 15:00 P2

Influence of sulfur doping on the creation yield of near-surface nitrogen vacancy centers and their charge state ratio — •Sven Graus[1], Ulrich Köhler[1], Tobias Lühmann[2], and Jan Meijer[2] — [1]Lehrstuhl für Experimentalphysik IV, Ruhr-Universität Bochum — [2]Felix-Bloch-Institut für Festkörperphysik, Angewandte Quantensysteme, Universität Leipzig

The negative charge state of nitrogen vacancy (NV) centers presents an extremely attractive candidate for a number of applications in quantum information technology and magnetometry. However, the implantation of near-surface NV centers shows a low yield and they have the tendency to convert into the neutral charge state. Recently, a significant increase in the creation yield of negative NV centers in the bulk of the diamond has been achieved by prior local doping of sulfur. We report on the in-situ implantation of sulfur and subsequent nitrogen implantation at energies of up to 5 keV while the sample is heated to temperatures of up to ∼800 °C under UHV conditions. Our setup presents a unique method for the implantation of near surface NV centers in small laboratories. First results on how these parameters influence the creation yield of negative NV centers close to the surface are presented.

KFM 25.4 Thu 15:00 P2

Improved thermoelectric properties of SnSe through forming a phase employing metavalent bonding — •Nan Lin, Yuan Yu, Oana Cojocaru-Miredin, and Matthias Wuttig — I.Physikalisches Institut IA, RWTH Aachen, Sommerfeldstraße 14, 52074 Aachen, Germany

SnSe only shows high ZT values above 750 K when the structure transforms from the asymmetrical Pnma phase to the higher symmetrical Cmcm phase. As a typical IV-VI compound bonded by p-state electrons, the Cmcm phase SnSe with an improved symmetry is expected to show the same chemical bonding with other rock-salt IV-VI compounds, which could be responsible for its excellent thermoelectric performance. Yet, it is challenging to stabilize the Cmcm phase at room temperature to characterize the bonding indicators. We successfully obtained the high-symmetry rock-salt SnSe phase by growing (SnSe)0.67(AgSbTe2)0.33, (SnSe)0.67(AgBiTe2)0.33, (SnSe)0.67(AgBiSe2)0.33, and (SnSe)0.5(AgSbSe2)0.5 alloys in a Bridgman oven. All cubic SnSe alloys show a unique portfolio of properties including a high optical dielectric constant, a large Born effective charge, and abnormal bond-breaking behavior in laser-assisted atom probe tomography. All these characteristics are indicative of the metavalent bonding mechanism while are not found in the pristine SnSe. Concomitantly, zT increases from near 0.1 for the Pnma SnSe to about 1.0 for all the Fm-3m SnSe phases. Our work demonstrates that metavalent bonding could be the origin of many special properties of SnSe including the excellent thermoelectric performance.

KFM 25.5 Thu 15:00 P2

Real space texture analysis using the 3D pair distribution function on a Pt thin film — •Sani Y. Harouna-Mayer[1,2], ZiZhou Gong[3], Martin v. Zimmermann[4], Ann-Christin Dippel[4], Simon J.L. Billinge[2], and Dorota Koziej[1,2] — [1]Institute for Nanostructure and Solid-State Physics, Center for Hybrid Nanostructures (CHyN), University of Hamburg, Hamburg, Germany — [2]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — [3]Department of Applied Physics and Applied Mathematics, Columbia University, New York, USA — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

An approach is described for studying texture in nanostructured materials. It is demonstrated on a fiber textured polycrystalline Pt thin film. The approach uses 3D PDF methods to reconstruct the orientation distribution function (ODF) of the powder crystallites from a set of diffraction patterns taken at different tilt angles of the substrate with respect to the incident beam directly from the 3D PDF of the sample. A real space equivalent of the reciprocal space pole figure is defined in terms of interatomic vectors in the PDF and computed for various interatomic vectors in the Pt film. Further, it is shown how a valid isotropic PDF may be obtained from a weighted average over the tilt series. Finally, we describe an open source Python software package, FouriGUI, that may be used to help in studies of texture from 3D reciprocal space data, and indeed for Fourier transforming and visualizing 3D PDF data in general.

KFM 25.6 Thu 15:00 P2

An X-ray diffraction studies on AlCrVY(O)N thin films. — •Eric Schneider[1], Michael Paulus[1], Nelson Filipe Lopes Dias[1], David Kokalj[2], Dominic Stangier[2], and Wolfgang Tillmann[2] — [1]Fakultät Physik/DELTA TU Dortmund University, 44221 Dortmund, Germany — [2]Institute of Materials Engineering, Dortmund, Germany

The aim of this project is to gain a fundamental understanding of the dependence between deposition parameters, layer structure and oxidation behavior of AlCrVY(O)N coatings. For this purpose, the coating systems were deposited on a WC-Co composite substrate by DC sputtering and high-energy pulse magnetron sputtering (HiPIMS). In addition to this, individual process parameters such as BIAS voltage and substrate temperature are varied to determine their influence on the thin films structure. For the investigation of the samples we used synchrotron radiation at beamline BL9 of the synchrotron radiation source DELTA (Dortmund, Germany) to perform XRD measurements. The samples were heated in an heating cell to temperatures up to 1000°C to study their oxidation behavior. Depending on the process parameters, different oxidation behaviour and residual stresses present in the samples were observed. We thank DELTA for providing synchrotron radiation. This work was supported by the DFG via TO 169/21-1.

KFM 25.7 Thu 15:00 P2

Hydrostatic high-pressure cells for X-ray scattering applications — •Kevin Lehninger[1], Christian Sternemann[1], Michael Paulus[1], Bridget Murphy[1], Metin Tolan[1], and Lutz Feldmann[2] — [1]Fakultät Physik/DELTA TU Dortmund, 44221 Dort-

mund, Deutschland — [2]Fakultät Physik/Konstruktionsbüro TU Dortmund, 44221 Dortmund, Deutschland

Small angle and wide angle X-ray scattering (SAXS/WAXS) at moderate pressures are of increasing relevance for the study of e.g. protein denaturation and stimuli responsive materials, respectively. One of the experimental challenges here is the precise pressure control in the pressure range up to 10 kbar while separating the sample volume from the pressure transmitting medium. For this purpose, we present two dedicated hydrostatic high pressure cells designed for use at beamlines BL2 and BL9 of the DELTA synchrotron radiation source that use water for pressure transmission. The WAXS cell with an opening angle of 60 degrees allows a sample volume with a cross-sectional area of one square millimeter that can be exposed to a maximum pressure of 5000 bar. The sample volume is enclosed in a flexible capillary tube which is placed between two diamond windows and can have a maximum diameter of 1.5 mm. The SAXS cell can be operated up to a pressure of 10000 bar providing an opening angle 20 degrees. Here the sample volume is contained in a cylinder sealed by polyimide film which is screwed into the high pressure cell by a slide system.

KFM 25.8 Thu 15:00 P2

Entwicklung von Herstellungsverfahren für koordinatenbasierte 3D Mikro-Standarts — •Celina Hellmich[1], Sebastian Bütefisch[1], Thomas Weimann[1], Stefanie Kroker[1,2] und Matthias Hemmleb[3] — [1]Physikalisch-Technische Bundesanstalt Braunschweig, Bundesallee 100, 38116 Braunschweig, Deutschland — [2]Technische Universität Braunschweig, Institut für Halbleitertechnik, LENA Laboratory for Emerging Nanometrology, Hans-Sommer-Str. 66, 38106 Braunschweig, Deutschland — [3]point electronic GmbH Erich-Neuß-Weg 15 D-06120 Halle (Saale) Deutschland

3D-Normale vereinen die Eigenschaften der üblichen Normale und die Kalibrierfaktoren für alle Achsen und die Kopplungsfaktoren zwischen ihnen können in einem Mess- und Auswertungsschritt ermittelt werden können. Mit diesem alternativen Kalibrieransatz können geometrische Verlagerungen über 3D-Referenzstrukturen mit bekannten Objektkoordinaten bestimmt werden. Die derzeit verwendeten 3D-Normale werden mit FIB hergestellt. Jedes Normal ist daher eine kostenintensive Sonderanfertigung, die zudem eine zeitaufwändige Kalibrierung erfordert. Daher sollen waferbasierte Maskenprozesse zur Herstellung von 3D-Standarts entwickelt werden, mit denen viele Strukturen reproduzierbar hergestellt und an das jeweilige zu kalibrierende Gerät angepasst werden können. Erste Ergebnisse wurden durch den schrittweisen Aufbau von Siliziumoxidschichten in Kombination mit einem Trockenätzverfahren erzielt. Auf diese Weise können zweistufige Pyramidenstrukturen hergestellt werden, auf die der Marker für die Kalibrierung mit Hilfe von Lift-off aufgebracht werden kann.

KFM 25.9 Thu 15:00 P2

The Relation between Electrocaloric Effect and Non-Collinear Electric Fields: A Coarse-Grained Case Study of $BaTiO_3$ — •Lan-Tien Hsu[1,2], Frank Wendler[1], and Anna Grünebohm[2] — [1]Institute of Materials Simulation (WW8), Friedrich-Alexander University of Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany

Ferroelectric perovskites are promising candidates for future electrocaloric cooling devices due to their adiabatic temperature changes in varying external electric fields.[1,2] Recently, the origin of the inverse electrocaloric effect (ECE) has been discussed.[2,3,4] In this work, we do coarse-grained molecular dynamic simulation using feram[5] to explore the phase stability and caloric responses of $BaTiO_3$ over a wide temperature range including fields in low-symmetry directions. We observe large inverse ECEs close to high-symmetry directions where the applied fields stabilize phases outside the zero-field coexistence temperature range. We believe this finding can provide general insights into the anisotropic nature of the ECE of ferroelectric perovskites.

[1] A. Torelló and E. Defay, Adv. Electron. Mater. (2022)
[2] A. Grünebohm, *et al.*, Energy Technol. **6** (2018)
[3] H. H. Wu and R. E. Cohen., J. Phys.: Condens. Matter **29** (2017)
[4] M. Marathe, *et al.*, Phys. Rev. B **96** (2017)
[5] T. Nishimatsu, *et al.*, Phys. Rev. B **78** (2008)

KFM 25.10 Thu 15:00 P2

Dielectric loss measurements of CVD diamond disks for ITER windows — •Sabine Schreck[1], Gaetano Aiello[1], Pablo Estebanez[2], Andreas Meier[1], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]F4E, Josep Pla 2, Torres Diagonal Litoral B3, 08019 Barcelona, Spain

Diamond disks manufactured by chemical vapor deposition (CVD) are essential elements of windows of the Electron Cyclotron Heating and Current Drive systems of fusion reactors like ITER. Diamond is selected as window material because of its high mechanical stability, high thermal conductivity and low dielectric loss. Only diamond disks with a low loss tangent guarantee a high transmission, i.e. a low absorption of microwave power in the disk. The latter results in moderate window temperatures and therefore in low thermal stresses. Hence, the measurement of the loss tangent is essential for the qualification of diamond disks for high-power windows. Dedicated measurement facilities (Fabry-Perot resonators) at KIT allow a high resolution measurement of the loss tangent at the disk centre (spherical set-up) as well as a mapping over the disk area to estimate its homogeneity (hemispherical set-up). Within a contract between F4E and KIT more than 60 diamond disks (D=70mm, t=1.11mm) produced similarly by MPA-CVD need to be qualified for their application in the ITER EC-system. The development of a dedicated test plan as well as initial results for the first disks delivered to KIT will be presented.

KFM 25.11 Thu 15:00 P2

X-ray emission spectroscopy at DELTA — •Nicola Thiering, Christian Albers, Robin Sakrowski, Michael Paulus, Metin Tolan, and Christian Sternemann — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

The analysis of the electronic and structural properties of transition metals is of enormous importance for a variety of research fields and applications. At beamline BL2 of the DELTA synchrotron radiation source (Dortmund, Germany) we used a hardened white beam of a bending magnet for efficient excitation to conduct X-ray emission spectroscopy experiments. The emission spectra were measured using a von Hámos spectrometer equipped with four cylindrically bent analyzer crystals in combination with a Pilatus 100K area detector. In order to demonstrate the capabilities of this setup, we present Kα, Kβ, and valence-to-core spectra of selected transition-metal bearing compounds.

KFM 25.12 Thu 15:00 P2

Phase retrieval for X-ray in-line holographic imaging: beyond the homogeneous object assumption — •Jens Lucht[1], Simon Huhn[1], Leon Merten Lohse[1,2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Universität Göttingen — [2]Deutsches Elektronen-Synchrotron DESY

X-ray lensless near-field holographic imaging offers high resolution 3d imaging with spatial resolution down to the nanometer scale with wide applicability in biomedical imaging and material sciences. To access quantitative images, phase retrieval has to be performed on the recorded Fresnel diffraction patterns. This constitutes an ill-posed inverse problem where several reconstruction methods have been developed. For high resolution synchrotron experiments, computationally efficient algorithms are needed. Widely employed is the computationally efficient contrast transfer function (CTF) method proposed by P. Cloetens two decades ago [P. Cloetens et al., Appl. Phys. Lett. 75, 2912 (1999)], besides more demanding nonlinear Fresnel propagation based methods. The CTF relies upon linearization of the Fresnel propagation. Notwithstanding its tremendous success, CTF-based methods often assume a homogeneous or low absorbing object as prior. We propose a CTF-based scheme that could relax these restriction to applicability while keeping reconstruction stability and computational requirements comparable. First experiments indicate very promising results.

KFM 25.13 Thu 15:00 P2

X-ray emission setup to study electronic structure of iron bearing compounds *in situ* at high pressure and high temperature — •Nicola Thiering[1], Christian Albers[1], Robin Sakrowski[1], Max Wilke[2], Johannes Kaa[1,4], Hlynur Gretarsson[3,5], Martin Sundermann[3,5], Metin Tolan[1,6], and Christian Sternemann[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Dortmund, Germany — [2]Institut für Geowissenschaften, Universität Potsdam, Potsdam, Germany — [3]Deutsches-Elektronen-Synchrotron DESY, Hamburg, Germany — [4]European XFEL, Schenefeld, Germany — [5]Max Planck Institute for Chemical

Physics of Solids, Dresden, Germany — [6]Universität Göttingen, Göttingen, Germany

The determination of iron-bearing compounds' electronic structure under high pressure and temperature (HPHT) conditions is pivotal to understand the chemistry, physics and dynamics of the Earth's interior [1]. We present a setup for investigating the electronic structure of such compounds *in situ* at HPHT up to 80 GPa and 3000 K, achieved by using diamond anvils cells in combination with a double-sided laser heating setup [2,3] using (resonant) X-ray emission spectroscopy ((R)XES) and show results for α-Fe_2O_3 and $FeCO_3$. (R)XES spectra were acquired utilizing a wavelength-dispersive von Hámos spectrometer in combination with a Pilatus 100K area detector [4] at PETRA III. [1] B. Orcutt et al. Deep Carbon (2019) [2] C. Albers et al. PRB 105 085155 (2022) [3] G. Spiekermann et al. JSR, 27, 414 (2020) [4] C. Weis et al. JAAS 34, 384 (2019)

KFM 25.14 Thu 15:00 P2

X-ray off-axis holography using iterative phase retrieval and waveguide beam splitters — •Paul Meyer and Tim Salditt — Institute for X-ray Physics, Georg August University of Göttingen, Germany

Propagation based phase contrast imaging (PB-PCI) with hard X-rays has become a powerful technique to study weakly absorbing specimen. Iterative algorithms can for example make single cells in a hydrated environment visible by retrieving the phase shift induced by the sample [1].

As image contrast in PB-PCI data arises from phase curvature, the reconstruction of low-frequency signals is challenging. In practice, it often requires support constraints on the sample. This problem does not arise with off-axis holography. Here, information of the phase image is extracted through interference with an additional reference beam that can for example be generated by a beamsplitting waveguide [2].

We observed that introducing such a reference beam in simulations for PB-PCI accelerates convergence and improves accuracy of the iterative phase retrieval (RAAR). We aim to transfer the observed advantage to the practical application of off-axis holography at synchrotron imaging facilities.

[1] Krenkel et al. Three-dimensional single-cell imaging with X-ray waveguides in the holographic regime. Acta Cryst A 73, 282-292 (2017). [2] Fuhse et al. Waveguide-Based Off-Axis Holography with Hard X Rays. Phys. Rev. Lett. 97, 254801 (2006).

KFM 25.15 Thu 15:00 P2

Hierarchically Porous Carbon Derived from the Activation of Waste Chestnut Shells as High Performance Electrode Materials for Supercapacitor — •Ping Hong[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Yunnan University, Kunming, People's Republic of China

3D hierarchical porous carbon consisting of micropores, mesopores and macropores was successfully prepared through the activation of chestnut shell with potassium bicarbonate (KHCO3). The influence of KHCO3/chestnut shell ratio on the textural properties was carefully investigated. By optimizing the amount of KHCO3, 3D hierarchical porous carbon with high specific pore surface area (2298 m2 g-1) and high total pore volume (1.51 cm3 g-1) were achieved. When applying the as-prepared 3D hierarchical porous carbon as electrode materials for supercapacitors, a high specific electric capacity of 387 F g-1 was reached at a current density of 2 A g-1. The remarkable electrochemical performances are mainly attributed to the hierarchical porous structure with the high specific surface area and the eminent total pore volume. It suggests that this hierarchical porous carbon prepared by activated by using KHCO3 would have more promising foreground in the field of energy storage.

KFM 25.16 Thu 15:00 P2

Ni-SnO2 nanopore arrays as potassium-ion battery anodes — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-ion batteries (SIBs) represent an effective energy storage technology with potentially lower material costs than lithium-ion batteries. Here, we show the electrochemical performance of SIBs with electrode design at the nanoscale. Highly ordered three-dimensional (3D) self-supported Ni-TiO2 nanopore arrays (NiNPA@TiO2) with highly oriented nanoporous structures are fabricated using nanoimprited AAO templating technique and applied as nanostructured anodes for SIBs applications. Their large specific surface area can ensure a high capacity, and their highly oriented and stable nanoporous structure can facilitate ion transport. The NiNPA@TiO2 nanoarrays delivered a reversible capacity of 240 mAh g-1 after 100 cycles at the current density of 50 mAh g-1 and were able to retain a capacity of 105 mAh g-1 at the current density as high as 5 A g-1. Their large active sites, high ion accessibility, fast electron transport, and excellent electrode integrity were shown as great merits to obtain the presented electrochemical performance. Not limited to the SIBs electrodes, the highly ordered 3D heterostructured nanoarrays as a promising electrode design for other electrochemical energy conversion and storage devices.

KFM 25.17 Thu 15:00 P2

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — •Jiajia Qiu[1,2], Huaping Zhao[1], Wenhui Ma[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Nanostructures of silicon are gradually becoming hot candidate due to outstanding capability for trapping light and improving conversion efficiency of solar cell. In this work, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of graphene-silicon (Gr-Si) solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs and Gr-SiIPs solar cells were systematically analyzed. The results show that the inverted pyramid arrays have more excellent ability for balancing antireflectance loss and surface area enlargement. The power conversion efficiency (PCE) and carrier lifetime of Gr-SiIPs devices respectively increase by 62% and 34% by comparing with that of Gr-SiNWs solar cells. Finally, the Gr-SiIPs cell with PCE of 5.63% was successfully achieved through nitric acid doping. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

KFM 25.18 Thu 15:00 P2

Structural behavior of delithiated $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ ($0<x<1$) battery cathodes — •Tobias Hölderle[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[2] — [1]Lehrstuhl für funktionelle Materialien, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany

The development of portable electronic devices up to electric vehicles powered with lithium-ion batteries led to an increased demand for lithium-ion batteries with higher capacities, energy/power densities, and cycling life. One of the most encouraging and state of the art commercial cathode materials are mixed lithium Ni, Co, Al metal oxides, e.g. in the form of high nickel content $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) cathodes possessing high energy and power densities at lower costs. Besides advantages, NCA materials possess several essential drawbacks. For example, NCA cathode materials are known to suffer from poor thermal stability, pronounced capacity as well as power density fading, and antisite disorder in NCA materials [1]. In the current contribution, a systematic *ex-situ* neutron powder diffraction study on differently electrochemically delithiated NCA cathode materials is presented. A set of structural parameters was obtained using full-profile Rietveld refinement. The lithium occupations reflect the increasing state-of-charge whilst the occupations of transition metals do not change, indicating the absence of antisite defects (cation mixing) in the NCA material. [1] C. Xu, P. J. Reeves, Q. Jacquet and C. P. Grey, Adv. Energy Mater., 11, 2003404 (2021).

KFM 25.19 Thu 15:00 P2

Dense binary Fe-Cu sites promoting CO2 utilization to enable highly-reversible hybrid Na-CO2 battery — •Changfan Xu — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — School of Metallurgy and Environment, Central South University, Changsha 410083, China — Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, Kunming 650093, China

A well-defined morphology of nitrogen-rich graphitic carbon frame-

work with dense bimetallic active sites (Fe-Cu-N-C) was facilely prepared by introducing Fe3+ and Cu2+ to regulate in-situ grown carbon nanotubes as an advanced catalyst toward hybrid Na-CO2 batteries. Through metal content-tuning and carbon architecture-altering, the Fe-Cu-N-C was proved to be dramatically more effective than Cu-N-C and Fe-N-C. As the cathodic catalyst of a hybrid Na-CO2 battery, Fe-Cu-N-C can facilitate the fast evolution and degradation of flocculent discharge products and achieve an excellent long-term cyclability up to 1550 cycles (over 600 h). The outstanding performance is attributed to the cross-linked conductive framework affording a highway for accelerating electron transport and Na+/CO2 diffusion. Besides, the synergistic effects among defect-rich interfaces, Fe/Fe3C nanocrystals, Fe-Nx, and Cu-Nx sites derived from nitrogen doping enhance the catalytic activity. The possible growth and decomposition mechanisms of NaHCO3 products were also presented and discussed.

KFM 25.20 Thu 15:00 P2

Dynamics of lithium-distribution in 18650-type LFP|C lithium-ion batteries during electrochemical cycling — •Dominik Petz[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Technische Universität München, Garching, Germany

The electrochemical cycling of lithium-ion batteries is characterized by an active transport of lithium ions and electrons, which are exchanged between the cathode and anode materials. Ionic exchange influences structural and chemical properties of electrode materials, which, in turn, affects electrode dimensions and geometry, current density, temperature, pressure, reaction rate, etc. Such parameters are in general neither uniformly nor statically distributed and therefore serve as stabilizing factor for heterogeneous states in lithium-ion batteries, which are typically reflected in the lithium concentration distribution in the electrodes. In most of the studies reported in literature, the lithium distribution has typically been examined in static equilibrium (e.g. in fully charged state), neglecting the evolution of the distribution under real charging conditions like the influence of C-rates, etc.

In this work the evolution of the lithium-ion distribution in the graphite anode was investigated in-operando by spatially-resolved neutron powder diffraction. Neutron data were supplemented by diffraction studies with high-energy photons. The occurrence of lithium inhomogeneities on different length scales was observed and will be presented in the current contribution.

KFM 25.21 Thu 15:00 P2

Strong electron-phonon coupling in $EuPd_2Si_2$ — •Mai Ye[1], Mark Joachim Graf von Westarp[1], Sofia-Michaela Souliou[1], Marius Peters[2], Robert Möller[2], Kristin Kliemt[2], Cornelius Krellner[2], and Matthieu Le Tacon[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

Mixed-valence metal $EuPd_2Si_2$ exhibits a valence transition from Eu^{2+} to Eu^{3+} with the crossover temperature T_v around 140 K [Jpn. J. Appl. Phys. 50 (2011) 05FD03]. On cooling, the tetragonal crystal symmetry is unchanged, with the a-axis length decreasing and the c-axis length essentially unchanging [arXiv:2203.05136]. We study the phonon modes of this material by Raman spectroscopy to explore the effect of valence transition and electron-phonon coupling. The Raman-active A_{1g} phonon mode shows Fano-type asymmetric lineshape, indicating interaction between the phonon mode and underlying continuum of electronic excitations. This mode also exhibits large frequency hardening on cooling: the frequency at 25 K is around 30% larger than that at 300 K. Such a large frequency change cannot be solely explained by the change of lattice parameters, which is only 2%, and points to the role played by electron-phonon interaction. Moreover, the frequency and linewidth of other Raman-active phonon modes show anomalies at T_v. We also present Raman spectra of $EuPd_2(Si_{0.94}Ge_{0.06})_2$ for comparison.