MLZ User Meeting 2021

Report of Contributions

Contribution ID: **1** Type: **Talk**

Hidden Charge Order in an Iron Oxide Square-Lattice Compound

Tuesday, December 7, 2021 4:15 PM (25 minutes)

Since the discovery of charge disproportionation in the FeO_2 square-lattice compound $Sr_3Fe_2O_7$ by Mössbauer spectroscopy more than fifty years ago, the spatial ordering pattern of the disproportionated charges has remained "hidden" to conventional diffraction probes, despite numerous x-ray and neutron scattering studies. We have used neutron Larmor diffraction and Fe K-edge resonant x-ray scattering to demonstrate checkerboard charge order in the FeO_2 planes that vanishes at a sharp second-order phase transition upon heating above 332 K. Stacking disorder of the checkerboard pattern due to frustrated interlayer interactions broadens the corresponding superstructure reflections and greatly reduces their amplitude, thus explaining the difficulty of detecting them by conventional probes. We discuss the implications of these findings for research on "hidden order" in other materials.

Primary author: PEETS, Darren (Technische Universität Dresden)

Co-authors: Dr KIM, Jung-Hwa (Max-Planck-Institut für Festkörperforschung); Dr REEHUIS, Manfred (HMI Berlin); Dr ADLER, Peter (MPI-CPfS); Dr MALJUK, Andrey (IFW-Dresden); Dr RITSCHEL, Tobias (Technische Universität Dresden); Dr ALLISON, Morgan (Technische Universität Dresden); Prof. GECK, Jochen (Technische Universität Dresden); Dr MARDEGAN, Jose (PETRA-III, DESY); Dr BERECIARTUA PEREZ, Pablo (PETRA-III, DESY); Dr FRANCOUAL, Sonia (PETRA-III, DESY); Dr WALTERS, Andrew (Max-Planck-Institut für Festkörperforschung); KELLER, Thomas (MPI for Solid State Research, Stuttgart); Dr ABDALA, Paula (ESRF); Dr PATTISON, Philip (ESRF); Mr DOSANJH, Pinder (University of British Columbia); Prof. KEIMER, Bernhard (Max-Planck-Institut für Festkörperforschung)

Presenter: PEETS, Darren (Technische Universität Dresden)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **2** Type: **Invited talk**

Magnetic field destroys long-range magnetic order in the Cu₂GaBO₅ ludwigite

Tuesday, December 7, 2021 9:05 AM (25 minutes)

The quantum spin systems Cu₂MBO₅ (M = Al, Ga) with the ludwigite crystal structure consist of a structurally ordered Cu²⁺ sublattice in the form of three-leg ladders, interpenetrated by a structurally disordered sublattice with a statistically random site occupation by magnetic Cu²⁺ and nonmagnetic Ga³⁺ or Al³⁺ ions. A microscopic analysis based on density-functional-theory calculations for Cu₂GaBO₅ reveals a frustrated quasi-two-dimensional spin model featuring five inequivalent antiferromagnetic exchanges. A broad low-temperature ¹¹B nuclear magnetic resonance points to a considerable spin disorder in the system. In zero magnetic field, antiferromagnetic order sets in below T_N ≈ 4.1 K and ~2.4 K for the Ga and Al compounds, respectively. From neutron diffraction, we find that the magnetic propagation vector in Cu₂GaBO₅ is commensurate and lies on the Brillouin-zone boundary in the (H0L) plane, q_m = (0.45, 0, −0.7), corresponding to a complex noncollinear long-range ordered structure with a large magnetic unit cell. Muon spin relaxation is monotonic, consisting of a fast static component typical for complex noncollinear spin systems and a slow dynamic component originating from the relaxation on low-energy spin fluctuations. Gapless spin dynamics in the form of a diffuse quasielastic peak is also evidenced by inelastic neutron scattering. Most remarkably, application of a magnetic field above 1 T destroys the static long-range order, which is manifested in the gradual broadening of the magnetic Bragg peaks. We argue that such a crossover from a magnetically long-range ordered state to a spin-glass regime may result from orphan spins on the structurally disordered magnetic sublattice, which are polarized in magnetic field and thus act as a tuning knob for field-controlled magnetic disorder.

Primary authors: KULBAKOV, Anton (TU Dresden); Dr SARKAR, Rajib (TU Dresden); Dr JANSON, Oleg (IFW Dresden); DENGRE, Shanu (TU Dresden); Dr MOSHKINA, Evgenia (Kirensky Institute of Physics, Krasnoyarsk, Russia); PORTNICHENKO, Pavlo (TU Dresden); Dr LUETKENS, Hubertus (Paul Scherrer Institute, Villigen, Switzerland); YOKAICHIYA, Fabiano (Helmholtz-Zentrum-Berlin); SUKHANOV, Aleksandr (TU Dresden); Dr EREMINA, Rushana (Zavoisky Physical-Technical Institute, Kazan, Russia); SCHNEIDEWIND, Astrid; Prof. KLAUSS, Hans-Henning (TU Dresden); INOSOV, Dmytro (TU Dresden)

Presenter: INOSOV, Dmytro (TU Dresden)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **3** Type: **Talk**

Stable DOPG/glycyrrhizin vesicles with a wide range of mixing ratios: Structure and stability as seen by scattering experiments and cryo-TEM

Tuesday, December 7, 2021 2:05 PM (25 minutes)

This study investigates the role of charged lipids in the plasma membrane with respect to the interaction of the antiviral saponin glycyrrhizin with such membranes. Glycyrrhizin is a natural triterpenic-based surfactant found in licorice. Vesicles made of 1,2-dioleoyl-sn-glycero-3-phospho-rac-(1'-glycerol) (DOPG)/glycyrrhizin are characterized by small-angle scattering with neutrons and X-rays (SANS and SAXS). Small-angle scattering data are first evaluated by the model-independent modified Kratky–Porod method and afterwards fitted by a model describing the shape of small unilamellar vesicles (SUV) with an internal head-tail contrast. Complete miscibility of DOPG and glycyrrhizin was revealed even at a ratio of lipid:saponin of 1:1. This is in line with the observation of glycyrrhizin not being haemolytic. Additional information about the chain-chain correlation distance of the lipid/saponin mixtures in the SUV structures is obtained from wide-angle X-ray scattering (WAXS).

Primary authors: Dr DARGEL, Carina (WWU Münster); GRÄBITZ-BRÄUER, Friederike; Dr GEISLER, Ramsia (Uniklinikum Frankfurt); FANDRICH, Pascal (Universität Bielefeld); Dr HANNAPPEL, Yvonne (Universität Bielefeld); Dr PORCAR, Lionel (ILL); Prof. HELLWEG, Thomas (Universität Bielefeld, PCIII)

Presenter: Prof. HELLWEG, Thomas (Universität Bielefeld, PCIII)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **4** Type: **Talk**

Critical fluctuations in the layered ruthenates Ca2RuO4 and Ca3Ru2O7

Tuesday, December 7, 2021 9:55 AM (25 minutes)

Materials realizing the scaling behavior of the XY model in two dimensions (2D) are sparse. Here we report on comprehensive neutron triple-axis measurements conducted at the FRM2, BER2, and ILL to investigate the critical static and dynamical magnetic fluctuations in the layered ruthenates Ca_2RuO_4 (CRO214) and $Ca_3Ru_2O_7$ (CRO327). Specifically, we probe the temperature-dependence of the antiferromagnetic (AFM) Bragg-intensity, the Q-width, the amplitude, and the energy-width of the magnetic diffuse scattering in vicinity to the Neel temperature T_N to determine the critical behaviour of the magnetic order parameter M, correlation length ξ, susceptibility χ, and the characteristic energy Γ. We find that - in spite of distinct magnetic structures - the critical behaviours of CRO214 and CRO327 follow similar universal scaling laws that are compatible with predictions of the 2D-XY model. Hence, our results suggest that single- and bilayer ruthenates provide new platforms to study the 2D-XY model in solid-state materials.

Primary authors: TREPKA, Heiko; KELLER, Thomas (MPI for Solid State Research, Stuttgart); KRAUTLOHER, Maximilian (Max Planck Institute for Solid State Research); HABICHT, Klaus (Helmholtz-zentrum Berlin für Materialien und Energie); XU, Jianhui (Helmholtz-Zentrum Berlin for Materials and Energy); BOEHM, Martin (Institut Laue-Langevin); KEIMER, Bernhard (Max Planck Institute for Solid State Research); HEPTING, Matthias (Max Planck Institute for Solid State Physics)

Presenter: TREPKA, Heiko

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **5** Type: **Talk**

Adhesion Process of Biomimetic Myelin Membranes Triggered by Myelin Basic Protein

Tuesday, December 7, 2021 1:40 PM (25 minutes)

The myelin sheath is an essential part of the nervous system, which enables rapid signal conduction. Damage of this complex membrane system results in demyelinating diseases such as multiple sclerosis (MS). The process in which myelin is generated in vivo is called myelination. In our study, we investigated the adhesion process of large unilamellar vesicles with a supported membrane bilayer that was coated with myelin basic protein (MBP) using time-resolved neutron reflectometry. Our aim was to mimic and to study the myelination process of membrane systems having either a lipid-composition resembling that of native myelin or that of the standard animal model for experimental autoimmune encephalomyelitis (EAE), which represents MS-like conditions. We were able to measure the kinetics of the partial formation of a double bilayer in those systems. The kinetics could be modelled using a random sequential adsorption simulation. By using a free energy minimization method, we were able to calculate the shape of the adhered vesicles and to determine the adhesion energy per MBP. For the native membrane the resulting adhesion energy per MBP is larger than that of the EAE modified membrane type. Our observations might help in understanding myelination and especially remyelination - a process in which damaged myelin is repaired - which is a promising candidate for treatment of the still mostly incurable demyelinating diseases such as MS.

Krugmann et al. (2021) Front. Chem. 9:631277

Primary authors: KOUTSIOUMPAS, Alexandros (JCNS); KRUGMANN, Benjamin (Forschungszentrum Jülich - JCNS 1); STADLER, Andreas (FZ Jülich); RADULESCU, Aurel (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ); Dr LAIREZ, Didier (CEA & CNRS); HARIS, Luman (Forschungszentrum Jülich); Dr MICCIULLA, Samantha (Institut Laue Langevin); FÖRSTER, Stephan (Forschungszentrum Jülich)

Presenter: STADLER, Andreas (FZ Jülich)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **6** Type: **Poster**

Tuning ordered mesoporous titania films via introducing germanium nanocrystals for high-efficient photoanodes

Tuesday, December 7, 2021 10:30 AM (1h 30m)

With an aim of obtaining high-efficient titania photoanodes, we introduce germanium nanocrystals (GeNCs) into a diblock-copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) template-assisted sol-gel synthesis. The surface and inner morphologies of the TiO2/GeNC films with different GeNC content after thermal annealing are investigated via scanning electron microscopy and grazing incidence small-angle X-ray scattering (GISAXS). GISAXS provides important insights into the influence of GeNC addition on the structure evolution. We probe the crystal phase, chemical state and optical properties of the nanocomposite films via X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy and ultraviolet-visible spectroscopy. These measurements show that even with GeNC addition, the nanocomposite films still have good crystallinity and high transparency. We further study the charge-carrier dynamics of the nanocomposite films. Compared to pristine titania photoanodes, the GeNC addition enhances the electron transfer, resulting in an overall improvement in the short-circuit current density (Jsc) of the exemplary perovskite solar cells and thereby an enhanced solar cell efficiency. The findings reveal that an optimal morphology is obtained by adding 2.5 wt% GeNCs, showing the largest pore sizes inside films. The optimized structures obtained in 2.5 wt% GeNCs yields, correspondingly, the best device performance.

Primary author: LI, Nian

Co-authors: GUO, Renjun (Physics E13, Technical University in Munich); CHEN, Wei (Technische Universität München); KÖRSTGENS, Volker (TU München); HEGER, Julian; LIANG, Suzhe (Physical Department, TUM); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: LI, Nian

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **7** Type: **Poster**

Aescin incorporation and nano-domain formation in DOPG model membranes observed by small-angle neutron scattering as well as small-angle and wide-angle X-ray scattering

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The saponin aescin can be extracted from the horse chestnut tree and is known for its anti-inflammatory and anti-oedematous properties. Using small, unilamellar lipid vesicle (SUV) as model membrane, we study the mixing properties of aescin with the phospholipid 1,2-dioleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (DOPG) by using small-angle neutron scattering (SANS), small- and wide-angle X-ray scattering (WAXS, SAXS). Due to the very low phase transition temperature of DOPG at T_m=-18 ℃ only the fluid like phase of the lipid is accessible. For pure DOPG vesicles SANS, SAXS and WAXS measurements lead to the expected vesicle like form factor. In SANS measurements the interaction of aescin is almost not visible in the form factor whereas in SAXS measurements the interaction leads to a significant change in the form factors. With SANS and SAXS measurements combined the dimension of the lipid bilayer is resolvable. In contrast, the chain-chain correlation in the bilayer is observable with WAXS measurements. The interaction of aescin with DOPG can be differentiated into two regimes which are based on the aescin concentration. For concentrations up to 10 mol% aescin is incorporated into the bilayer statistically. For concentrations from 20-50 mol% a nano-domain formation of aescin can be assumed in the bilayer. The nano-domain formation is observable by a change in the SANS and SAXS form factors as well as the appearance of a second chain-chain distance in the WAXS signal.

Primary author: GRÄBITZ-BRÄUER, Friederike

Co-authors: DARGEL, Carina (Bielefeld University); GEISLER, Ramsia (Uniklinikum Frankfurt); FANDRICH, Pascal (Universität Bielefeld); HANNAPPEL, Yvonne (Universität Bielefeld); PORCAR, Lionel (ILL); SCHWEINS, Ralf (Institut Laue - Langevin); HELLWEG, Thomas (Universität Bielefeld, PCIII)

Presenter: GRÄBITZ-BRÄUER, Friederike

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **8** Type: **Talk**

Resonant neutron reflectometry for hydrogen detection in thin films.

Tuesday, December 7, 2021 9:05 AM (25 minutes)

The study of hydrogen diffusion and storage in different materials is crucial in the challenge of an actual implementation of sustainable energy sources, but also to explore the possible modification of electronic, magnetic and optical properties of the host materials. Due to high sensitivity of neutrons to hydrogen atoms, neutron scattering techniques have been successfully used for many decades. Neutron reflectometry in particular is demonstrated to be a powerful method for the study of hydrogen absorption in thin films for atomic concentrations of 5% and higher. In this talk we will show a new model-free method which allows to measure smaller (<5%) concentrations of hydrogen absorbed in situ, with smaller counting times and with a higher sensitivity. The method is based on measuring the position of the resonance formed due to the contrast between the optical potential of a layer and its neighbours. Hydrogen absorption leads to a change of this optical potential and hence to a shift of the resonance position. We will present experiments conducted on Al2O3/Nb(x)/Co(3nm)/Nb(x)/Pt(3nm) thin films demonstrating that hydrogen concentrations below 1% and absorption kinetics of few seconds can be measured using this method.

Primary author: GUASCO, Laura

Co-authors: KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research); PÜTTER, Sabine (Jülich Centre for Neutron Science JCNS, Outstation at MLZ, Forschungszentrum Jülich GmbH); KELLER, Thomas (MPI for Solid State Research, Stuttgart); PAULIN, Mariano Andrés (Comisión Nacional de Energía Atómica); SILVI, Luca (Helmholtz-Zentrum Berlin); KEIMER, Bernhard (Max Planck Institute for Solid State Research)

Presenter: GUASCO, Laura

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **9** Type: **Poster**

Tailoring the Optical Properties of Sputter-Deposited Gold Nanostructures on Nanostructured Titanium Dioxide Templates

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Au/TiO2 nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. We use customized polymer templating to achieve TiO2 nanostructures with different morphologies. Au/TiO2 hybrid thin films are fabricated by sputter deposition. An in-depth understanding of the Au morphology on the TiO2 templates is achieved with in situ GISAXS during the sputter deposition. The resulting Au nanostructure is largely influenced by the TiO2 template morphology. Based on the detailed understanding of the Au growth process, characteristic distances can be selected to achieve tailored Au nanostructures at different Au loadings. For selected sputter-deposited Au/TiO2 hybrid thin films, the optical response with a tailored localized surface plasmon resonance is demonstrated.

Primary authors: Prof. FAUPEL, Franz (LS Materialverbunde, Institut für Materialwissenschaft, CAU); Mr DREWES, Jonas (LS Materialverbunde, Institut für Materialwissenschaft, CAU); YIN, Shanshan; LIANG, Suzhe (Physical Department, TUM); GENSCH, Marc; SCHWARTZKOPF, Matthias (DESY); Mr CARSTENS, Niko (LS Materialverbunde, Institut für Materialwissenschaft, CAU); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); SCHAPER, Simon; ROTH, Stephan (DESY / KTH); Dr STRUNSKUS, Thomas (LS Materialverbunde, Institut für Materialwissenschaft, CAU); CHEN, Wei (Technische Universität München)

Presenter: LIANG, Suzhe (Physical Department, TUM)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **10** Type: **Talk**

Fast kinetics in thin films by intensity modulated neutron reflectometry

Tuesday, December 7, 2021 9:30 AM (25 minutes)

We propose a method for kinetic neutron reflectometry with a time resolution of a few μs. The method is based on periodic excitation of the sample and phase locked modulation of the beam intensity by one radio frequency spin flipper, and requires a position sensitive neutron detector with time resolution also in the order of 1 μs. The output are time resolved reflectivity curves locked to the phase of the sample excitation parameter. The method is compatible with polarization analysis and off-specular scattering. Thus, lateral and depth resolved chemical and magnetic SLD (scattering length density) profiles can be measured with the aforementioned time resolution. Future applications are, for example, the study of spintronic thin film devices based on implanted hydrogen, where small shifts of the hydrogen concentration profiles induced by a gating voltage can dramatically effect magnetic, electric, and superconducting properties.

Primary author: KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research)

Co-authors: KELLER, Thomas (MPI for Solid State Research, Stuttgart); GUASCO, Laura; Prof. KEIMER, Bernhard

Presenter: KELLER, Thomas (MPI for Solid State Research, Stuttgart)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **11** Type: **Talk**

Studying the uniformity of custom-made Li-ion pouch cells using operando neutron powder diffraction and spatially resolved synchrotron X-ray diffraction

Tuesday, December 7, 2021 9:55 AM (25 minutes)

A custom-made, multilayered Li-ion battery pouch cell was investigated using operando neutron powder diffraction (NPD) and spatially resolved powder X-ray diffraction (SR-PXRD) with the aim of comparing the information obtained from the two complementary techniques. The work focused on the anode and cathode lithiation as obtained from the LiC6/LiC12 weight ratio and the NMC111 c/a-ratio, respectively. Using a rotary stage, Rietveld refineable neutron powder diffractograms were measured with geometrical effects minimized. Using SR-PXRD, the cell was shown to be non-uniform in its anode and cathode lithiation, with the edges of the cell being less lithiated/delithiated than the center. This was more pronounced for high charging current than low charging current. The averaged SR-PXRD data was found to match the bulk NPD data well. This is encouraging as it seems to allow comparisons between studies using either of these complimentary techniques. This work will also serve as a benchmark for our future studies on pouch cells with novel noncommercial cathode and/or anode materials.

Primary author: SØRENSEN, Daniel (MLZ)

Co-authors: HEERE, Michael; SENYSHYN, Anatoliy; BARAN, Volodymyr (DESY, FS-PETRA-D, P02.1)

Presenter: SØRENSEN, Daniel (MLZ)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **12** Type: **Poster**

Multi-scale phase quantification of strain-induced martensite in Austempered Ductile Iron (ADI) using different neutron diffraction techniques

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Austempered ductile iron (ADI) is an attractive material with excellent mechanical properties, like high strength, good ductility, wear resistance and fatigue strength. Its mechanical properties are largely determined by the ausferritic microstructure which contains retained high carbon enriched austenite. The retained austenite will become unstable under plastic deformation and will transform to strain-induced martensite. Because of plastic deformation and similar crystal structure of martensite and ferrite, the quantitative phase analysis of the strain-induced martensite in ADI using diffraction techniques has two difficulties, i.e., texture formation and peaks overlapping. These difficulties will influence the accuracy of quantitative phase analysis. By means of different neutron diffraction techniques and methods, like standard Rietveld method using whole diffraction pattern (SPODI + STRESS-SPEC) including the texture effect, texture method from the measured pole figure intensity (STRESS-SPEC) and Bragg edge neutron transmission method (Antares), the difficulties in phase quantification were will be presented in current contribution. Furthermore, the advantages, disadvantages and accuracy of each method will be discussed and summarized.

Primary author: LI, Xiaohu (FRM2, Physik, TU München)

Co-authors: Dr SORIA, Sergio (FRM II); GAN, Weimin (Helmholtz-Zentrum Hereon); HOFMANN, Michael; HOELZEL, Markus; SCHULZ, Michael

Presenter: LI, Xiaohu (FRM2, Physik, TU München)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **13** Type: **Poster**

GISANS study on whey protein and titania interfaces: Influence of pH on spray deposited biohybrid film morphology

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Interfaces based on metal oxides play a major role in functional materials for energy applications. For example, TiO2 can serve as a photocatalyst in the production of hydrogen or as an anode material in emerging solar cell and battery technologies. In most applications, a designed structure is highly de-sired to fulfill performance conditions on different length scales. Moreover, devices benefit from a high interfacial area between functional layers and hence nanostructured TiO2 of high surface-to-volume ratio is favorable. Designed morphologies can be achieved and fabricated by industrial rele-vant, low-cost solution processing, e.g. spray deposition, with the help of diblock copolymer directed sol-gel synthesis. However, involved organic solvents limit the potential in environmentally friendly processing when it comes to an industrial scale. To overcome this, synthetic copolymers can be re-placed by water-soluble biopolymers. The bovine whey protein forms aggregates of different structures by denaturing at different pH values that can act as a template in water-based TiO2 synthesis. Different biohybrid films are obtained by spray deposition from the solutions at different pH. The films are in-vestigated with bulk and surface-sensitive grazing-incidence small-angle neutron scattering (GISANS) to understand the influence of pH on the morphology. The obtained results are complemented by real-space imaging.

Primary author: Mr HEGER, Julian E. (TUM Physik E13)

Co-authors: Mrs GEIGER, Christina (TUM Physik E13); Dr KREUZER, Lucas P. (TUM Physik E13); Mr WIDMANN, Tobias (TUM Physik E13); Mrs YIN, Shanshan (TUM Physik E13); Dr KOUTSIOUMPAS, Alexandros (JCNS-MLZ); Prof. MÜLLER-BUSCHBAUM, Peter (TUM Physik E13, MLZ)

Presenter: Mr HEGER, Julian E. (TUM Physik E13)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **14** Type: **Poster**

A Unique Quenching and Deformation Dilatometer for Combined In Situ Neutron Diffraction Analysis of Engineering Materials

Wednesday, December 8, 2021 10:30 AM (1h 30m)

A modified quenching and deformation dilatometer (TA instruments DIL 805A/D/T) is now in operation at the Heinz Maier-Leibnitz Zentrum (MLZ, Germany) neutron center. It is customized for running neutron scattering measurements during the temperature/deformation treatment of the sample, in particular neutron diffraction (phase, texture, and lattice strain) and neutron small angle scattering. The bulk length change of dilatometer specimens is successfully combined with in situ neutron diffraction patterns for analyzing dynamic processes in metallic materials. A detailed introduction to the unique dilatometer is given and examples of recent experiments highlight the use of the added insight provided by combining diffraction and dilatometry.

Primary author: LI, Xiaohu (Forschungs-Neutronenquelle FRM II)

Co-authors: SOLIS, Cecilia; GAN, Weimin (Helmholtz-Zentrum Hereon); HOFMANN, Michael; LANDESBERGER, Martin (TUM); Mr REIBERG, Marius (Institute of Materials Science and Mechanics of Materials Technische Universität München)

Presenter: LI, Xiaohu (Forschungs-Neutronenquelle FRM II)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **15** Type: **Poster**

Functionalizing cellulose nanofibril films

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Cellulose nanofibrils (CNF), extracted from wood, are sustainable materials par excellence and used to fabricate high-strength materials. A promising route for fabricating porous CNF films on large scale is spray deposition using water-based technologies; the resulting porous CNF templates are excellent candidates to infiltrate conductive polymers and plasmon-active nanoparticles for functionalization. This functionalization is based on adding additional layers or depositing CNF-based dispersions using solvent-based methods; often, the solvent itself is water. With CNF being hygroscopic, it is therefore mandatory to understand the interaction of water with the CNF films. We employ in situ grazing incidence small-angle neutron scattering to study the morphological features within the ultra-smooth CNF thin films under as-prepared conditions as well as their rearrangement under humidification. In a next step, we used poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), widely applied in organic photovoltaics and electronics, to functionalize the CNF template. We studied the infiltration, resulting structural rearrangement within the thin CNF template of, and their behavior under cyclic humidity changes by grazing incidence small-angle neutron scattering. Extending to plasmonic applications, we employ layer-by-layer deposition of laser-ablated silver nanoparticles to install a plasmon-active CNF-template.

Primary authors: ROTH, Stephan (DESY / KTH); Dr BRETT, Calvin (KTH & DESY); Prof. SÖDERBERG, Daniel (KTH); FRIELINGHAUS, Henrich (JCNS); Prof. MANSSON, Martin (KTH); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr CHEN, Qing (DESY)

Presenter: ROTH, Stephan (DESY / KTH)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **16** Type: **Talk**

Cracking during high temperature deformation of a high-strength polycrystalline Co-base superalloy

Tuesday, December 7, 2021 1:40 PM (25 minutes)

The polycrystalline Co-base superalloy CoWAlloy1 provides a high potential for high temperature applications as wrought alloy due to a high γ' precipitate fraction and γ/γ' lattice misfit which lead to excellent creep properties. However, cracking occurs during hot rolling. Therefore, this study investigated the origins of crack formation during processing.
Compression tests at temperatures between 1000–1150 ℃ and different strain rates were executed to characterize the deformation at high temperatures. The formed cracks were analyzed by scanning electron microscopy (SEM). An intercrystalline crack propagation could be revealed if cracking occurred. The tendency of crack growth decreases with increasing temperature. Apparently, the precipitation of γ' phase and the absent recrystallization lead to pronounced crack propagation below the γ' solvus temperature. In-situ high temperature small-angle neutron scattering (SANS) helped to understand the phase fractions and precipitate size distributions at different processing temperatures. A low γ' volume fraction is present at the heat treatment temperature of 1075 ℃ while a high fraction of γ' precipitates forms during cooling to 750 ℃. In consequence, the material provides a high strength when the hot bar encounters with the cold rolls during hot rolling due to the high amount of γ' phase in the rim of the bar and thus cracking starts there. Instead of that, the strength is decreased and crack growth is minimized at 1075 ℃.

Primary authors: HAUSMANN, Daniel (Friedrich-Alexander-Universität Erlangen-Nürnberg); Dr FREUND, Lisa (Friedrich-Alexander-Universität Erlangen-Nürnberg); Dr SOLÍS, Cecilia (German Engineering Materials Science Center (GEMS)); Prof. GÖKEN, Mathias (Friedrich-Alexander-Universität Erlangen-Nürnberg); Dr GILLES, Ralph (Heinz Maier-Leibnitz Zentrum (MLZ)); Dr NEUMEIER, Steffen (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Presenter: HAUSMANN, Daniel (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **17** Type: **Talk**

Capturing the catalytic proton of dihydrofolate reductase: implications for general acid-base catalysis

Tuesday, December 7, 2021 9:30 AM (25 minutes)

Acid-base catalysis, which involves one or more proton transfer reactions, is a chemical mechanism commonly employed by many enzymes. The molecular basis for catalysis is often derived from structures determined at the optimal pH for enzyme activity. However, direct observation of protons from experimental structures is quite difficult; thus, a complete mechanistic description for most enzymes remains lacking. Dihydrofolate Reducatse (DHFR) exemplifies general acid-base catalysis, requiring hydride transfer and protonation of its substrate, DHF, to form the product, tetrahydrofolate (THF). Previous X-ray and neutron crystal structures coupled with theoretical calculations have proposed that solvent mediates the protonation step. However, visualization of a proton transfer has been elusive. Based on a 2.1 Å resolution neutron structure of a pseudo-Michaelis complex of E. coli DHFR determined at acidic pH, we report the direct observation of the catalytic proton and its parent solvent molecule. Comparison of X-ray and neutron structures elucidated at acidic and neutral pH reveals dampened dynamics at acidic pH, even for the regulatory Met20 loop. Guided by the structures and calculations, we propose a mechanism where dynamics are crucial for solvent entry and protonation of substrate. This mechanism invokes the release of a sole proton from a hydronium (H3O+) ion, its pathway through a narrow channel that sterically hinders the passage of water, and ultimate protonation of DHF at the N5 atom.

Primary author: WAN, Qun (Nanjing Agricultural University)

Co-authors: Dr KOVALEVSKY, Andrey (Oak Ridge National Lab); Dr BENNETT, Brad (Biological and Environmental Science Department, Samford University); Dr BROOKS, Charles (Department of Chemistry, University of Michigan); Dr DEALWIS, Chris (Case Western Reserve University); Dr PAUL, Langan (Oak Ridge National Lab); Dr WILSON, Mark (Department of Biochemistry and Redox Biology Center, University of Nebraska); Dr WYMORE, Troy (Department of Chemistry, University of Michigan); Dr LI, Zhihong (Nanjing Agricultural University)

Presenter: WAN, Qun (Nanjing Agricultural University)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **18** Type: **Talk**

Neutron coating development applied to non-depolarizing CuTi supermirrors

Tuesday, December 7, 2021 9:55 AM (25 minutes)

In the last two years we improved our understanding of sputtering process parameters leading to (Ni,Ti) supermirror coatings with reduced mechanical stress and higher reflectivity. This knowledge has been applied to the case of non-depolarizing m=2 (Cu,Ti) supermirrors, which have been successfully prepared with the standard DC magnetron sputtering facility of the FRM II neutron optics group. Control on the roughness grow and interdiffusion allowed us to get a very good maximum angle of total reflection (ca. 0.21°/λ) and neutron reflectivity (ca. 87%), with pure diamagnetic properties. Those characteristics make them suitable for experiments where a high non-depolarization factor is needed.

Primary author: Dr GOMEZ GUZMAN, Jose Manuel (Technische Universität München Heinz Maier-Leibnitz Zentrum (MLZ))

Co-author: LINK, Peter

Presenter: Dr GOMEZ GUZMAN, Jose Manuel (Technische Universität München Heinz Maier-Leibnitz Zentrum (MLZ))

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **19** Type: **Talk**

Optimization of the new testing machine for in-situ microstructural characterization under mechanical and thermal loading

Tuesday, December 7, 2021 4:40 PM (25 minutes)

The goal of the BMBF funded project HiMat is the optimization of an innovative testing machine to perform deformation experiments at high temperatures at various instruments at the research neutron source Heinz Maier-Leibnitz. With diffraction, small-angle scattering and radiography (tomography) it is possible to investigate forming phases, their volume fractions as well as size and shape, dislocation densities, textures, recrystallization processes and crack propagation.

The field of possible loading cases of the testing machine is manifold: uniaxial tensile and compression experiments, creep experiments and cyclic loading or crack propagation tests. The testing temperatures can be varied from room temperature up to 1200 ℃ and the tests can be performed in vacuum or defined atmospheres. Furthermore, a contactless measurement tool was implemented, which enables a spatial resolved temperature and strain measurement. Thus, the optimized testing machine represents a unique sample environment for the investigation of high-performance materials. This is demonstrated exemplarily with the Co-based superalloy CoWAlloy, which was developed by the FAU, and the Ni-based superalloy VDM® Alloy 780 in the HiMat project.

Primary authors: Dr KUEMMEL, Frank (Heinz Maier-Leibnitz Zentrum (MLZ), TU München); Mr DEEB, Osama (Hochschule München); Mr KIRCHMAYER, Andreas (Department of Materials Science & Engineering, FAU Erlangen-Nürnberg); Dr FRITTON, Massimo (Heinz Maier-Leibnitz Zentrum (MLZ), TU München); Dr NEUMEIER, Steffen (Department of Materials Science & Engineering, FAU Erlangen-Nürnberg); Dr GILLES, Ralph (Heinz Maier-Leibnitz Zentrum (MLZ), TU München)

Presenter: Dr KUEMMEL, Frank (Heinz Maier-Leibnitz Zentrum (MLZ), TU München)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **20** Type: **Invited talk**

Vibrational density of state of the ideal glass

Tuesday, December 7, 2021 9:05 AM (25 minutes)

The vibrational density of state (VDOS) of the most stable crystal of a given species follows the prediction of the Debye model. In contrast, glasses generally exhibit excess in the VDOS visible as a bump in the meV range and widely known as the boson peak. Its magnitude depends on the thermodynamic state of the glass. Specifically, the magnitude of the boson peak scales with the entropy and energy of the glass.

In the present contribution, we employ a model system of polymer nanospheres, where the thermodynamic state can be tuned at wish by manipulating the amount of free interface and the annealing time deep in the glassy state, to study the effect of deeply reducing the glass energy on the VDOS. In doing so, we show that, in appropriate conditions, the thermodynamic state of the glass can be reduced down to the condition of entropy matching that of the crystal. We show that in this state the boson peak of the glass is essentially suppressed and, therefore, the VDOS mimics that of the crystal. We interpret this results as a signature of the transformation of the glass into a new state, named “the ideal glass”, long ago theorized, whose existence is in this way demonstrated.

Primary author: CANGIALOSI, Daniele

Co-authors: COLMENERO, Juan (Centro de Fisica de Materiales CSIC-UPV/EHU); Dr MONNIER, Xavier (Donostia International Physics)

Presenter: CANGIALOSI, Daniele

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **21** Type: **Poster**

Effect of SEI formation on lithium diffusion coefficients in Si thin film anodes

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The solid electrolyte interphase (SEI) is a solid protective barrier that forms at the surface of lithium-ion batteries (LIB) operating outside the stability range of the electrolyte. In particular, that happens at the anode where Li metal reduces the liquid electrolyte forming a solid mixture of inorganic and organic components during the lithiation reaction [1]. A good barrier layer prevents further electrolyte decomposition and prevents the exfoliation of the anode material during cycling. However, if the SEI layer is unstable, it would lead to electrolyte loss, termed 'drying out', and increased electrode impedance. Both processes cause reduced efficiency and capacity fading [2]. Silicon has drawn the attention of researchers as one of the most outstanding alternate materials for the next generation of LIB anodes. It possesses a very high theoretical storage capacity (4200 mAh g−1) compared to all other known materials [3]. However, in addition to the large volume change during Li (de)intercalation process [4], the instability of the SEI layer is a dominant disadvantage of Si anode, which leads to capacity decline and poor kinetics [5]. To understand the effect of SEI on the lithium-ion transport rate in Si thin-film anodes, galvanostatic intermittent titration technique (GITT) measurements were performed on RF sputtered amorphous Si films. The main goal was to determine Li diffusivities with LiClO4-based and LiPF6-based liquid electrolytes at room temperature. It was found that lithium diffusion coefficients of Si in LiClO4-based electrolytes are higher during the Li intercalation process. Furthermore, the morphology, composition, and thickness of the SEI layer are found to be different in various electrolytes, which will lead to differences in lithium-ion diffusion coefficients. To further explore the effect of the SEI layer, in situ neutron reflectometry (NR) will be applied in the near future to continuously study the composition and thickness of the SEI layer in Si anodes during the (de)lithiation process.

Primary author: Mr WU, Baolin (RWTH Aachen University; Forschungszentrum Jülich (IEK-9))

Co-authors: Dr CHEN, Chunguang (Forschungszentrum Jülich (IEK-9)); Dr DANILOV, Dmitri L. (Forschungszentrum Jülich (IEK-9); Eindhoven University of Technology); Dr VEZHLEV, Egor (Forschungszentrum Jülich (JCNS-4)); Prof. EICHEL, Rüdiger-A. (RWTH Aachen University;Forschungszentrum Jülich (IEK-9)); Prof. NOTTEN , Peter H.L. (Forschungszentrum Jülich (IEK-9); Eindhoven University of Technology)

Presenter: Mr WU, Baolin (RWTH Aachen University; Forschungszentrum Jülich (IEK-9))

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **22** Type: **Talk**

Microstructure and Mechanical behavior of Mg-5Zn matrix influenced by Particle Deformation Zone via in situ neutron diffraction

Tuesday, December 7, 2021 2:05 PM (25 minutes)

Magnesium alloys have the advantages of low density, high specific strength and specific stiffness, so they have been widely used in many fields, such as aerospace, aerospace, automobile and electronic products, etc [1,2]. However, the application of magnesium alloys is limited because of the low modulus, low strength and poor plasticity at room temperature. In recent years, it has been found that the mechanical properties of magnesium alloys can be significantly improved by adding SiCp.
In this contribution the effect of particle deformation zone (PDZ) size on the microstructure and thus mechanical properties of SiCp/Mg-5Zn composites was studied. Furthermore, the work hardening and softening behavior of SiCp/Mg-5Zn composites influenced by PDZ size were analyzed and discussed using neutron diffraction under in-situ tensile deformation. Evolution of FWHM (full width at half maximum) extracted from the diffraction pattern of SiCp/Mg-5Zn composites was used to interpret the modification of dislocation density during in-situ tension, to elucidate their influence on the work hardening behavior of SiCp/Mg-5Zn composites.
A comprehensive overview on the deformation behavior of SiCp/Mg-5Zn composites will be given in this presentation. In particular, our results show that the work hardening rate of SiCp/Mg-5Zn composites increased with the enlargement of PDZ size, which was attributed the corresponding increase in grain size of composites. In addition, the stress reduction values increased continuously during in-situ tensile for SiCp/Mg-5Zn composites due to the stored energy produced during plastic deformation, which provided a driving force for softening effect.

Primary authors: HOFMANN, M. (Technische Universität München); Dr NIE, Kai-bo (Taiyuan University of Technology); Dr DENG, Kun-kun (Taiyuan University of Technology); Dr SHI, Quan-xin (Taiyuan University of Technology); Dr GAN, Wei-min (Helmholtz-Zentrum Hereon)

Presenter: Dr DENG, Kun-kun (Taiyuan University of Technology)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **24** Type: **Plenary talk**

Updates on the JCNS Deuteration Service - First Call for Proposals

Wednesday, December 8, 2021 4:25 PM (20 minutes)

Neutron scattering experiments involving soft matter materials often require specific contrast to observe different parts of the materials. In order to increase the availability of deuterium labelled materials, we are currently establishing deuteration support to MLZ users. Our main synthetic focus at the JCNS-1 is in the area of polymers and ethoxylation (e.g. surfactants). We have recently sent out a survey to the community to find out about the interest in our services and the results will be presented during this talk.

As we plan to publish the call for proposals directly after this meeting, this talk will also answer the following questions: Which kind of materials could you obtain from us? How can you get materials from us? Where can you submit your proposals? How will the proposals be evaluated? And what do we plan for the future?

Primary authors: FRUHNER, Lisa (JCNS-1, Forschungszentrum Jülich GmbH); ALLGAIER, Jürgen (FZ Jülich)

Co-author: FÖRSTER, Stephan (Forschungszentrum Jülich)

Presenter: FRUHNER, Lisa (JCNS-1, Forschungszentrum Jülich GmbH)

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **25** Type: **Poster**

Fast Neutron Imaging with Semiconductor Nanocrystal Scintillators

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Fast neutrons offer high penetration capabilities for both light and dense materials due to their comparatively low interaction cross-sections, making them ideal for the imaging of large-scale objects such as as-built plane turbines, for which X-rays or thermal neutrons do not provide sufficient penetration. However, inefficient fast neutron detection limits the widespread application of this technique. Traditional phosphors such as ZnS:Cu embedded in plastics are utilized as scintillators in recoil proton detectors for fast neutron imaging. However, these scintillation plates exhibit significant light scattering due to the plastic–phosphor interface along with long-lived afterglow (on the order of minutes), and therefore alternative solutions are needed to increase the availability of this technique. Here, we utilize colloidal nanocrystals (NCs) in hydrogen-dense solvents for fast neutron imaging. The light yield, spatial resolution, and neutron-vs-gamma sensitivity of several chalcogenide (CdSe and CuInS2)-based and perovskite halide-based NCs are determined, with only a short-lived afterglow (below the order of seconds) observed for all of these NCs. FAPbBr3 NCs exhibit the brightest total light output at 19.3% of the commercial ZnS:Cu(PP) standard, while CsPbBrCl2:Mn NCs offer the best spatial resolution at ~2.6 mm.

Primary authors: SAKHATSKYI, Kostiantyn (ETH Zurich, Empa); Dr YAKUNIN, Sergii (ETH Zurich, Empa); Prof. KOVALENKO, Maksym (ETH Zurich, Empa)

Co-authors: Dr MCCALL, Kyle (ETH Zurich); Dr LEHMANN, Eberhard (PSI); Dr WALFORT, Bernhard (RC Tritec AG); Dr LOSKO, Adrian (Technische Universität München, Forschungs-Neutronenquelle MLZ (FRMII)); Dr MONTANARELLA, Federico (ETH Zurich, Empa); Dr BODNARCHUK, Maryna (ETH Zurich, Empa); Dr KRIEG, Franziska (ETH Zurich, Empa); Dr KELESTEMUR, Yusuf (ETH Zurich, Empa); Dr MANNES, David (Paul Scherrer Institut); Dr SHYNKARENKO, Yevhen (ETH Zurich, Empa)

Presenter: SAKHATSKYI, Kostiantyn (ETH Zurich, Empa)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **26** Type: **Talk**

Nematic Correlation Length in Iron-Based Superconductors

Tuesday, December 7, 2021 4:40 PM (25 minutes)

Nematicity is ubiquitous in electronic phases of high-T_c superconductors, particularly in the Fe-based systems. We used inelastic neutron and x-ray scattering to extract the temperature-dependent nematic correlation length ξ from the anomalous softening of acoustic phonon modes in $Ba(Fe_{1-x}Co_x)_2As_2$ and FeSe. In all cases, we find that ξ is well described by a power law $(T–T_0)^{-1/2}$ extending over a wide temperature range. Combined with the previously reported Curie-Weiss behavior of the nematic susceptibility, these results point to the mean-field character of the nematic transition, which we attribute to a sizable nemato-elastic coupling that is likely detrimental to superconductivity.

Primary authors: Dr MERRITT, Adrian (Forschungszentrum Jülich); Prof. FERNANDES, Raphael (University of Minnesota); WEBER, Frank (Karlsruhe Institute of Technology); Prof. REZNIK, Dmitry (University of Colorado)

Co-authors: Dr ALATAS, Ahmet (Argonne National Laboratory); Dr BARON, Alfred (RIKEN SPring-8 Center); Dr SAID, Ayman (Argonne National Laboratory); Dr CASTELLAN, John-Paul (CEA Saclay)

Presenter: WEBER, Frank (Karlsruhe Institute of Technology)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **27** Type: **Poster**

Project CAESAR: Cell Chemistry Based on Silicon Anode and Nickel-Rich Cathode

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The new project CAESAR funded by the Bundesministerium für Wirtschaft und Energie (BMWi) is a cooperation of the Technical University Munich (TUM) including the FRM II and several industrial partners under the leadership of the company Wacker. The aim of this project is the development of Li ion batteries (LIB) with increased specific energy (Wh/kg) and energy density (Wh/l) accompanied by a decrease of the specific cost (€/Wh). To this end, an appropriate combination of high-capacity materials is substantial, in this case Si anodes and Ni-rich layered oxide cathodes. The project encompasses the whole value chain of LIBs from the material development to the validation of prototypes for applications. Thereby, neutron studies at the FRM II will help to analyze failure mechanisms of LIBs and reveal inherent processes to improve their performance. Neutrons are well suited for LIB research since measuring concentrations and distributions of light elements such as Li is feasible. Furthermore, the discriminability of neighboring elements in the periodic system with neutrons is essential here since the cathode materials contain Co, Mn as well as Ni. In this poster, the just-started CAESAR project and the associated neutron experiments will be introduced. Moreover, first neutron depth profiling (NDP) results of differently lithiated Si anodes will be presented. They reveal the distribution of Li throughout the anodes which has a major impact on their cycling stability.

Primary author: GROSSMANN, Lukas

Co-authors: Dr VACIK, Jiri; GILLES, Ralph

Presenter: GROSSMANN, Lukas

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **28** Type: **Poster**

Critical Review of symmetry and structure relationships in graphite intercalation compounds (GICs) and their practical use for lithium ion battery materials

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Graphite and materials made of graphite have historically been of huge technological importance due to their manifold interesting properties. High performance lithium-ion batteries (LIBs) typically use graphite-based anode materials. The energy storage is achieved through the reversible reaction of the graphite with lithium ions in an electrochemical intercalation reaction. When the material is completely transformed to the stage-1 compound with maximum lithium content, LiC6 is obtained. The transformation to LiC6 however is complex and between the two terminal points of this reversible reaction, many intermediate stages exist. The profound complexity and peculiarities of this "staging" reaction, especially in the Li-Graphite system however are not yet fully understood. Although a full understanding is imperative in order to control aging and cell performance characteristics of lithium ion batteries.
We have critically reviewed the existing binary stage-1 GIC structures and especially the Li-GIC structures from the ICSD-database. We review fundamental structural aspects like bonding distances and packing arrangements and explore their symmetry relationships applying group-subgroup considerations. Our findings can be used to improve the understanding of the intermediate stages occurring during the electrochemical intercalation of lithium ions in LIBs and to enhance the analysing of measured neutron data.

Primary authors: Dr SEIDLMAYER, Stefan (Technische Universität München, Heinz Maier-Leibnitz Zentrum (MLZ)); Dr SCHEURER, Christoph (Fritz-Haber-Institute, Max-Planck-Gesellschaft, Theory Department); GILLES, Ralph

Presenter: Dr SEIDLMAYER, Stefan (Technische Universität München, Heinz Maier-Leibnitz Zentrum (MLZ))

Session Classification: Poster Session II

Track Classification: Structure Research

Contribution ID: **29** Type: **Poster**

X-ray Diffraction Studies on the Lithiation of LiAl Electrodes for Lithium Ion Batteries

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Metal alloys as anode material for lithium ion batteries such as LiAl offer a high theoretical capacity in relation to their low cost. Compared to the conventional graphite anode, aluminium has an almost three times higher specific capacity with 993 mAh/g. During lithiation, aluminium first forms a solid solution with lithium called the alpha-LiAl phase until the solubility limit is reached. Subsequently, the alpha-LiAl will transform to the beta-LiAl upon further lithiation near the electrolyte-electrode interface.

Here, phase identification via x-ray diffraction (XRD) measurements was performed in order to help the understanding of the lithiation mechanism. First results have shown that both alpha-LiAl and beta-LiAl are present within the sample. Higher lithiated phases such as Al2Li3 could not be identified. For both SOC 25 and SOC 50 however, LiOH could be determined as an additional phase whereas the percentage was higher for samples charged to SOC 50. Similarly, a higher amount of beta-LiAl was identified while the samples charged to SOC 25 showed an increased percentage of alpha-LiAl. Operando XRD measurements are planned that will minimize the ambient air related formation of LiOH and allow the measurement of alpha- and beta-LiAl nucleation directly under protective conditions.

This work is performed as a collaboration between TUM (Heinz Maier-Leibnitz Zentrum, FRM II) and RWTH Aachen (ISEA) in the frame of the BMBF project ExcellBattMat cluster.

Primary author: Mr PHAM, Thien An (TU München, Heinz Maier-Leibnitz Zentrum (MLZ))

Co-authors: Mr WELLS, Luke (RWTH Aachen, Institut für Stromrichtertechnik und Elektrische Antriebe); SEIDLMAYER, Stefan (TU München, Heinz Maier-Leibnitz Zentrum (MLZ)); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); FIGGEMEIER, Egbert (RTWH Aachen, Institut für Stromrichtertechnik und Elektrische Antriebe); GILLES, Ralph (TU München, Heinz Maier-Leibnitz Zentrum (MLZ))

Presenter: Mr PHAM, Thien An (TU München, Heinz Maier-Leibnitz Zentrum (MLZ))

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **30** Type: **Talk**

Structural investigation of ferrofluids under external electric fields by neutron scattering

Tuesday, December 7, 2021 9:55 AM (25 minutes)

It is well known, the properties of magnetic fluids can be controlled by external magnetic field. However, inhomogeneous distribution of magnetic particles in non-polar ferrofluids was observed recently under external electric fields and formation of large aggregates was concluded in such systems. It was shown that aggregation process depends on the magnitude of the DC electric field, and in alternating electric fields with a frequency of more than 800 mHz, aggregates are not formed at all. Also, the detected anisotropy of the SANS signal at the detector indicates the preferred orientation of the aggregates of magnetic particles in ferrofluids. Impact of temperature on such aggregation was also checked by SANS and it was concluded that with temperature increase above 60 ℃, the aggregates formed in the electric field are destroyed. SANS with polarized neutrons was performed for detail study of the nuclear and magnetic structures in such systems. Behaviour of ferrofluids under external fields at different nanoparticles concentrations was investigated as well. The question of relaxation processes after switching off the field and returning the structure to its original state was considered.

Primary authors: FEOKTYSTOV, Artem; PETRENKO, Viktor (BCMaterials. Basque center for materials, applications & nanostructures); HONECKER, Dirk (ISIS Neutron and Muon Source); Mr KARPETS, Maksym (Institute of Experimental Physics SAS, Kosice, Slovakia); Dr RAJNAK, Michal (Institute of Experimental Physics SAS, Kosice, Slovakia); Dr AVDEEV, Mikhail (Joint Institute for Nuclear Research, Dubna, Russia); Dr TIMKO, Milan (Institute of Experimental Physics SAS, Kosice, Slovakia); Dr KOPCANSKY, Peter (Institute of Experimental Physics SAS, Kosice, Slovakia); PIPICH, Vitaliy

Presenter: PETRENKO, Viktor (BCMaterials. Basque center for materials, applications & nanostructures)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **31** Type: **Poster**

QENS study of the diffusivity of hydrogen in MoS2

Tuesday, December 7, 2021 10:30 AM (1h 30m)

With an increase in renewable energy production, the problem of energy storage becomes more and more significant. One of the most promising ideas is storage in form of hydrogen gas, which involves the production of hydrogen by electrolysis and later its reconversion into electricity in fuel cells. It is of great importance for these processes to be carried out most efficiently with the most readily accessible materials. Therefore, there have been intense studies in the search for catalyst materials for the hydrogen and oxygen evolution reactions.
Molybdenum disulphide, MoS_2, has shown promising behaviour as a catalyst in the hydrogen evolution reaction (HER), which is completely in line with its known activity for hydrogenation reactions. In this presentation we will show the results of our study of the diffusion of hydrogen adsorbed inside layered MoS_2 crystals, for which we used quasi-elastic neutron scattering, neutron spin-echo spectroscopy, nuclear reaction analysis, and X-ray photoelectron spectroscopy \[1\]. The neutron measurements demonstrate fast diffusion of hydrogen molecules parallel to the basal planes of MoS_2. A much slower hydrogen diffusion was observed perpendicular to the basal planes using nuclear reaction analysis.
1 V. Kuznetsov, W. Lohstroh, D. Rogalla, H-W. Becker, T. Strunskus, A. Nefedov, E. Kovacevic, F. Traeger and P. Fouquet, Physical Chemistry Chemical Physics 23 (2021) 7961 – 7973.

Primary authors: KUZNETSOV, Vitalii (Institut Laue Langevin); Prof. TRAEGER, Franziska (Westfälische Hochschule); FOUQUET, Peter (Institut Laue-Langevin)

Co-authors: LOHSTROH, Wiebke; Dr ROGALLA, Detlef (RUBION, Ruhr-Universität Bochum); Dr BECKER, Hans-Werner (RUBION, Ruhr-Universität Bochum); Dr STRUNSKUS, Thomas (Technische Fakultät der Universität Kiel); Dr NEFEDOV, Alexei (Karlsruher Institut für Technologie (KIT)); Prof. KOVACEVIC, Eva (Université d'Orléans)

Presenter: KUZNETSOV, Vitalii (Institut Laue Langevin)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **32** Type: **Poster**

Dynamics of lithium-concentration in 18650-type lithium-ion batteries during electrochemical cycling

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Electrochemical cycling of lithium-ion batteries is supplemented by the active transport of lithium ions and electrons, which are exchanged between the cathode and anode material. Besides material properties, such exchange is facilitated by cell parameters like electrode dimensions and geometry, current density, temperature, pressure, reaction rate etc. Such parameters are neither uniformly distributed nor static in general and, therefore, serve as stabilizing factor of heterogeneous states in Li-ion batteries typically reflected in the lithium concentration distribution in the electrodes [1, 2].
In most studies reported in the literature the lithium distribution was typically probed in the static equilibrium (for example in the fully charged state in the graphite anode), neglecting the evolution of the distribution under real charging conditions, influence of C-rates etc.
In this work, the evolution of the lithium-ion distribution in the graphite anode was studied in operando using spatially-resolved neutron powder diffraction. Neutron data were complemented by diffraction studies using high energy photons; occurrence of lithium inhomogeneities on different length scales and their dynamics was observed and will be presented in current contribution.

1. Senyshyn, A., et al., Homogeneity of lithium distribution in cylinder-type Li-ion batteries. Scientific Reports, 2015. 5(1): p. 18380.
2. Petz, D., et al., Heterogeneity of Graphite Lithiation in State-of-the-Art Cylinder-Type Li-Ion Cells. Batteries & Supercaps, 2021. 4(2): p. 327-335.

Primary author: PETZ, Dominik

Co-authors: MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); SENYSHYN, Anatoliy

Presenter: PETZ, Dominik

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **33** Type: **Talk**

Calculation of neutron and X-Ray scattering data from Molecular Dynamics simulations through optimal use of computation resources

Tuesday, December 7, 2021 4:15 PM (25 minutes)

Optimization of computation time has always been a challenge in the world of computation. In this work, we address the computation of X-Ray and neutron scattering data from molecular dynamics simulations. There are multiple software solutions available for this; we have chosen sassena for our work. Sassena inherits distributed memory parallelization (MPI) from its previous version. This work further augments vectorization and shared memory parallelization (OpenMP) into it and bolsters the computing speed of sassena. Furthermore, the introduction of shared memory parallelization introduces a possibility of doing hybrid parallelization. As a long term goal, we aim to use the benefit of this optimization to validate the simulation of hydrogen storage materials with neutron scattering data.
Keywords:
1) Parallel computing
2) Neutron scattering
3) Molecular Dynamics Simulation
4) sassena

Primary author: MAJUMDAR, Arnab (Helmholtz Zentrum hereon)

Co-authors: Prof. MÜLLER, Martin (Institute of Materials Physics, Helmholtz-Zentrum Hereon); Dr BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon)

Presenter: MAJUMDAR, Arnab (Helmholtz Zentrum hereon)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **34** Type: **Poster**

Investigations on the kinetics of the liquid-liquid phase separation of myelin basic protein: Combining neutron scattering with imaging techniques

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The myelin basic protein (MBP) is a key player when it comes to the formation of tight membrane wrapping around vertebrate's nerve cells. In physiological conditions, MBP is acting as a glue that stacks multiple myelin layers to build up an insulating sheath which covers axons. To accomplish this task, MBP undergoes a so-called Liquid-Liquid Phase Separation (LLPS) - a property which has recently attracted wide attention in the biological and biophysical community. In a LLPS, two liquid phases with different protein concentrations and physio-chemical properties coexist. Damaged integrity of human MBP and the consequent lack of LLPS capability often results in neurodegenerative diseases such as, for instance, Multiple Sclerosis.
Although the importance of its ability to perform a LLPS is already known, the kinetics of MBP's phase separation are not well studied yet. Hence, we focus on investigations that follow the formation of liquid-like MBP droplets which can be observed when suitable conditions are applied. To examine both the nucleation and the growth of those µm-sized condensates, we combine imaging techniques and (neutron) scattering experiments: Confocal microscopy of labelled MBP has confirmed the phase separation and provided information about the droplet size distribution. These finding we compared to Small Angle Neutron Scattering (SANS) experiments in a q-range of $7 \cdot 10^{-5} - 6 \cdot 10^{-1}$ Å^{-1}. Microfluidic experiments where combined with high-speed camera imaging in order to obtain details about the nucleation kinetics. Complementary, a stopped flow setup was used for Time Resolved (TR-SANS) experiments to support the previous results and to determine the growing droplet size within low second to early minute time-scale in situ. For long term droplet growth, Dynamic Light Scattering (DLS) yielded a $t^{1/3}$-dependent growth which indicates Ostwald ripening as dominating mechanism.

Primary author: GRAF VON WESTARP, Igor

Co-author: STADLER, Andreas (FZ Jülich)

Presenter: GRAF VON WESTARP, Igor

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **35** Type: **Talk**

Chirality of Bloch domain walls in exchange biased CoO/Co bilayer seen by waveguide-enhanced neutron spin-flip scattering

Tuesday, December 7, 2021 1:15 PM (25 minutes)

The magnetic state of exchanged biased CoO(20nm)/Co(d_F) bilayers (d_F=5-20nm) was studied by means of polarized neutron reflectometry. By introducing a Nb(20nm) spacer layer between the CoO/Co bilayer and the Al_2O_3 substrate, we designed a resonator structure with significantly enhanced intensity of the spin-flip (SF) scattering at the position of the optical resonances. For the trained sample with thinnest Co layer (d_F = 5nm), we detected strong SF scattering at the resonance position to the amount of 30\% the incoming intensity, pointing to a high degree of non-collinearity of the magnetization. With increasing d_F, the intensity of the SF scattering decreases linearly. Furthermore, an unconventional asymmetry of up-down and down-up scattering channels at the resonance positions was observed, which we ascribe to the out-of-plane magnetic stray field generated by chiral Bloch domain walls. This field leads to Zeeman splitting of the neutron energies depending on the initial neutron spin polarization. The chirality of the domain walls is assigned to Dzyaloshinskii-Moriya interaction emerging at the CoO/Co interface. Our observations might prove useful for the design of spintronic devices based on the exchange bias effect.

Primary authors: SIDORENKO, A. (Institute of Electronic Engineering and Nanotechnologies ASM, MD2028 Kishinev, Moldova); LENK, D (Institut für Physik, Universität Augsburg); KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research); KEIMER, Bernhard (Max-Planck-Institut für Festkörperforschung); TAGIROV, L. (Institut für Physik, Universität Augsburg); MORARI, R. (Institut für Physik, Universität Augsburg); TIDECKS, R. (Institut für Physik, Universität Augsburg); HORN, S. (Institut für Physik, Universität Augsburg); KELLER, Thomas (MPI for Solid State Research, Stuttgart); ZDRAVKOV, V. (Institut für Physik, Universität Augsburg)

Presenter: KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **36** Type: **Talk**

Overcoming the challenges of residual stress analysis by neutron diffraction in additively manufactured alloys

Tuesday, December 7, 2021 1:15 PM (25 minutes)

Metal Additive manufacturing (AM) technologies such as Laser Powder Bed Fusion (LPBF) enable the fabrication of complex structures, giving rise to potential improvements in component and manufacturing efficiency. However, the processes are typically characterized by the generation of high magnitude residual stresses which can have detrimental consequences for subsequent applications. Therefore, the characterization of these residual stress fields and understanding of their formation and mitigation through optimized processing is crucial for the wider uptake of the technology. Due to the potential complex nature and high value of components manufactured by LPBF, it is important to have suitable characterisation methods which can determine the spatial variations of RS in a non-destructive manner. Neutron diffraction is considered to be the best suited for these requirements. However, the microstructures developed in the complex thermal cycles experience in the production can pose challenges to the ND method for residual stress analysis. The BAM has conducted significant research over the past years to overcome these obstacles, enabling higher confidence in the residual stresses determined in LPBF materials by neutron diffraction. This contribution will overview some of these advancements made recently at European neutron sources including on Stress-Spec at FRM2/MLZ.

Primary authors: Dr EVANS, Alexander (Bundesanstalt für Materialforschung und –prüfung (BAM)); ULBRICHT, Alexander; Dr KROMM, Arne (Bundesanstalt für Materialforschung und –prüfung (BAM)); BRUNO, Giovanni (Bundesanstalt für Materialforschung und –prüfung (BAM)); Dr SERRANO-MUNOZ, Itziar (Bundesanstalt für Materialforschung und –prüfung (BAM)); Mr SCHRÖDER, Jakob (Bundesanstalt für Materialforschung und –prüfung (BAM)); Mr SPRENGEL, Maximilian (Bundesanstalt für Materialforschung und -prüfung); Dr MISHUROVA, Tatiana (Bundesanstalt für Materialforschung und –prüfung (BAM)); Prof. KANNENGIESSER, Thomas (Bundesanstalt für Materialforschung und –prüfung (BAM)); Dr FRITSCH, Tobias (Bundesanstalt für Materialforschung und –prüfung (BAM))

Presenter: Dr EVANS, Alexander (Bundesanstalt für Materialforschung und –prüfung (BAM))

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **37** Type: **Poster**

Na-ion diffusion in NASICON solid electrolyte material studied by Quasi-Elastic Neutron Scattering

Wednesday, December 8, 2021 10:30 AM (1h 30m)

The sodium superionic conductor (NASICON) materials have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries due to their high conductivity and facile synthesis conditions. The aim of this work is to elucidate the reason for extremely high conductivity exhibited by some compositions, specifically by $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}(0 \text{ x } 3)$. We investigate the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at ≈170℃, on the Na-ion occupancy in the crystal structure. Additionally, we study the influence of other dopant elements (Sc and Y) on the Na^+ ionic conductivity. Quasi-elastic neutron scattering (QENS) is used to measure spatial and temporal dynamic properties of diffusion of Na^+ ions in the crystal lattice. The measurements were performed at the BASIS spectrometer at the Spallation Neutron Source, Oak Ridge National Laboratory in Tennessee, USA. For the evaluation of the QENS data, the DAVE software (NIST Center for Neutron Research) is used. Important information about the Na^+ ion diffusion process, such as activation energies, jump distances between the occupation sites and characteristic times of jumps can be extracted from the measured QENS data. The detailed data analysis is still in progress. This worked was performed as a collaboration between TUM (Heinz Maier-Leibnitz Zentrum, FRM II) and Forschungszentrum Jülich (IEK-1) in the frame of the BMBF project ExcellBattMat cluster.

Primary author: PIVARNÍKOVÁ, Ivana

Co-authors: Dr SEIDLMAYER, Stefan; Dr FINSTERBUSCH, Martin (Forschungszentrum Jülich GmbH); Mr DÜCK, Geralt (Forschungszentrum Jülich GmbH); Dr NAQASH, Sahir (Forschungszentrum Jülich GmbH); Dr JALARVO, Niina (Neutron Scattering Division, Oak Ridge National Laboratory); Prof. MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr GILLES, Ralph

Presenter: PIVARNÍKOVÁ, Ivana

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **38** Type: **Talk**

X-ray and neutron studies on H-bonded polymers that help stabilize lithium metal anodes

Tuesday, December 7, 2021 9:05 AM (25 minutes)

Lithium metal batteries are next generation energy storage devices that rely on the stable electrodeposition of lithium metal during the charging process. In this work, we investigate the effect of polymer dynamics on lithium metal deposition. For this, we design electrolyte (solvent) blocking perfluoro polyether polymer networks with evenly spaced H-bonding sites of various strengths, resulting in significant differences in the molecular ordering, as analyzed by x-ray scattering measurements (SAXS and WAXS). The differences in the H-bonding strength directly influence the mechanical properties of these materials, thus providing a controlled set of samples with a range of polymer dynamics for electrodeposition studies. A systematic evaluation of the lithium metal electrodeposition quality with these polymers as anodic coating showed that polymers with flowability or faster polymer dynamics exhibited higher coulombic efficiency. Preliminary results on the polymer with the strongest H-bonding using the quasielastic neutron scattering (QENS) technique will be shown. The work was supported by the US-German joint collaboration on "Interfaces and Interphases In Rechargeable Li-metal based Batteries" supported by the US Department of Energy (DOE) and German Federal Ministry of Education and Research (BMBF).

Primary authors: Dr PAUL, Neelima (Technical University of Munich, Heinz Maier-Leibnitz Zentrum (MLZ)); Ms HUANG, Zhuojun (Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305); Dr CHOUDHURY, Snehashis; Mr THIENENKAMP, Johannes Helmut; LENNARTZ, Peter (Institute of Energy and Climate Research IEK-12: Helmholtz-Institute Münster (HI MS) Ionics in Energy Storage); GONG, Huaxin; WOLF, Marcell (TUM); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr BRUNKLAUS, Gunther (Institute of Energy and Climate Research, IEK-12: Helmholtz-Institute Münster (HI MS) Ionics in Energy Storage, Münster, Germany); GILLES, Ralph; Prof. BAO, Zhenan (Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305)

Presenter: Dr PAUL, Neelima (Technical University of Munich, Heinz Maier-Leibnitz Zentrum (MLZ))

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **39** Type: **Poster**

In-situ characterisation of the newly developed VDM® Alloy 780 via x-ray diffraction using synchrotron radiation

Wednesday, December 8, 2021 10:30 AM (1h 30m)

The new VDM® Alloy 780 is a Ni-based superalloy developed for higher service temperatures than the widely used alloy 718, consisting of γ matrix, γ´ hardening phase, and δ & η high-temperature phases. Depending on the respective heat treatment of VDM® Alloy 780, various microstructures with different phase proportions can be obtained, which determine the mechanical properties of the alloy over the entire application temperatures.
Via in-situ x-ray diffraction measurements at elevated temperatures, the dissolution of both the γ´ hardening phase and the high-temperature phases can be directly tracked, enabling to determine their solvus temperatures. Also, directly accessible from the measurements is the lattice misfit, i.e. the relative difference of lattice parameters of γ matrix and γ´ hardening phase, and its evolution with temperature which is decisive for the mechanical properties of the alloy and the morphology of the precipitates.
Due to the higher time resolution at the synchrotron, the obtained solvus temperature values are more accurate as previously published by neutron diffraction. However, neutron measurements have much better particle statistics due to the larger measured volume and an enlarged separation of peaks at high theta angles, corroborating the synergistic effect of combining both techniques. Therefore, the synchrotron diffraction data is analyzed comparatively to the existing neutron data.

Primary author: FRITTON, Massimo

Co-authors: Dr KÜMMEL, Frank (MLZ TUM); Dr HAFEZ, Masood (VDM Metals International GmbH); Dr GEHRMANN, Bodo (VDM Metals International GmbH); Dr GILLES, Ralph (MLZ TUM); SOLIS, Cecilia

Presenter: FRITTON, Massimo

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **40** Type: **Poster**

The influence of toluene in a Si/Ge sol-gel approach

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Latest research has revealed promising results for silicon (Si) and germanium (Ge) as anode materials for lithium-ion batteries (LIBs). Owing to their high energy capacity these two group 14 semiconductors are considered as auspicious alternatives to graphite anodes in LIBs. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a well-known wet chemical sol-gel approach. Here, the amphiphilic diblock copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) is used as the structuring agent. As the silicon/germanium source, novel soluble 29 atomic Zintl clusters (K12SixGe17-x) are used. In the experiment, we investigate the structural difference that occurs when toluene is used as an additive. Real-space data as SEM and microscopy images will be discussed with reciprocal-space analysis methods as grazing-incidence x-ray scattering in small-angle mode and powder x-ray diffraction data. The study is completed by energy-dispersive X-ray spectroscopy (EDS). As EDS mapping can only probe the surface, we are highly interested in the Si/Ge distribution in bulk. Neutron Scattering in grazing-incidence mode (GISANS) is a key factor in analyzing the inner composition of the thin film.

Primary authors: WEINDL, Christian L. (TU München, Physik-Department, LS Funktionelle Materialien); FAJMAN, Christian E. (TU München, Chemie-Department, Lehrstuhl für anorganische Chemie); FÄSSLER , Thomas F. (TU München, Chemie-Department, Lehrstuhl für anorganische Chemie); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: WEINDL, Christian L. (TU München, Physik-Department, LS Funktionelle Materialien)

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **41** Type: **Poster**

Co-Nonsolvency Transition of PNIPMAM-based Block Copolymer Thin Films in Water/Acetone Mixtures

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich phase in a certain range of compositions of these two solvents. The nonionic thermo-responsive polymer, poly(isopropylmethacrylamide) (PNIPMAM), which features a lower critical solution temperature (LCST) in aqueous solution, has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethyllammonio)butane-1-sulfonate)) (PSBP)□which exhibits an lower upper critical solution temperature (UCST) and shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPMAM thin films in water/acetone-d6 mixed vapors by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier Transform Infra-red (FTIR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which is closely related to their deuteration level.

Primary author: WANG, Peixi (Workgroup Polymer Interfaces, TUM Department of Physics, Technical University of Munich)

Co-authors: GEIGER, Christina (Technical University of Munich, Chair of Functional Materials); KREUZER, Lucas P. (TUM Physik E13); LIANG, Suzhe (Physical Department, TUM); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); REITENBACH, Julija; WIDMANN, Tobias (TU München, Physik Department, LS Funktionelle Materialien)

Presenter: WANG, Peixi (Workgroup Polymer Interfaces, TUM Department of Physics, Technical University of Munich)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **42** Type: **Poster**

Tack Properties of Pressure-Sensitive Adhesives: Development of Industry-conform Measurement Techniques

Wednesday, December 8, 2021 10:30 AM (1h 30m)

For the mechanical characterization of the adhesive bond of pressure-sensitive adhesives one has to take into account the geometry of the adherents and the kind of stress applied. We present a technique, which is especially adapted for the measurement of tack for assemblies of fibers coated with pressure-sensitive adhesives using customized cylindrical composite stamps 1. Key element of the method is the proposed technique to achieve monolayers of parallel-aligned fibers as a fiber assembly. With the adapted probe tack test we investigated the tack properties of a polymer blend of poly(vinylpyrrolidone-co-vinylacetate) and polyethylene glycol (PEG) coated on human hair. This composition serves as a simple model system for hair styling products. The influence of different PEG contents and of the humidity on the tack is demonstrated. 1 V. Körstgens et al., ACS Appl. Polym. Mater. 2, 3189-3195 (2020).

Primary author: KÖRSTGENS, Volker (TU München)

Co-authors: CORELLA PUERTAS, Jorge; MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: KÖRSTGENS, Volker (TU München)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **43** Type: **Poster**

Influence of Mg2+ on the structure and interface of all-solid-state lithium battery

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The interest in all-solid-state lithium batteries mainly originates from its high safety and energy density compared with conventional Li-ion batteries. Solid polymer electrolytes (SPEs) as an essential component with high durability, long shelf life, high energy density, great flexibility for cell design and low weight are considered as the most promising material for next generation batteries. However, as the most common SPE, poly(ethylene oxide) (PEO) electrolytes have a limited electrochemical window and can react with lithium metal to form a solid electrolyte interphase (SEI), meaning that such SPE is more instable in high-energy-density batteries. Moreover, inhomogeneity at the electrolyte/electrode interface can elicit an irregular lithium plating that leads to dendrite formation, resulting in the cycle life reduction and total cell resistance increase. As a modifying strategy, adding inorganic particles can alter the degree of non-conducting crystalline polymer volume within the electrolyte, promote the dissociation of Li+-TFSI- ion pairs and increase the amount of mobility Li+ ions. Herein, Mg(ClO4)2 is introduced to the electrolyte and a series of SPE-Mgx electrolyte(x ranges from 0.25 to 1) are fabricated to modify the structure of SPE and increase the ionic conductivity. Besides, the additive can also assist in constructing a Li+ conducting SEI at the electrolyte/electrode interface. The formation of SEI layer can be detected during cycling with neutron reflectometry in future measurements.

Primary author: Ms LIANG, Yuxin (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany)

Co-author: Prof. MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: Ms LIANG, Yuxin (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **44** Type: **Poster**

Interfacial structure and dynamics for PbS quantum dot solar cells

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Colloidal quantum dots (CQDs) have generated great interest in various optoelectronic devices because of their size-tunable bandgap, low-temperature solution processability. Lead sulfide (PbS) CQDs, with a strong absorption coefficient and large Bohr radius, enable solar cells to harvest infrared photons of the solar spectrum beyond the absorption edge of crystalline silicon and perovskites. There have been many strategies to improve device performance, among which interface engineering is a promising method. Excellent interface engineering is designed to form an energy cascade to enable an efficient charge transfer and promote exciton dissociation. Moreover, it can also offer good interfacial contact and improve device air stability by selecting appropriate materials. Here, we sputter the indium zinc oxide (IZO) as the interlayer between PbS QDs absorption layer and ZnO nanoparticle (NP) electron transport layer (ETL), to fabricate PbS QD solar cells and study the trap densities and charge transport process at QDs interfaces. In addition, we also study the dynamics process of how the IZO is sputtered on the ITO glass and ITO/ZnO respectively.

Primary authors: ZHONG, Huaying; MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); CHEN, Wei (Technische Universität München)

Presenter: ZHONG, Huaying

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **45** Type: **Poster**

Influence of Hofmeister Salts on the Swelling Behavior of PNIPMAM Thin Films

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Thermoresponsive polymer thin films have gained a lot of attention in the past decades due to their attractiveness for a wide range of applications. A variety of polymer showing LCST- or UCST-type behavior are known, and their transition temperatures can be influenced by various factors such as molar mass, end groups, copolymerization, or by the addition of salts. For polymers in aqueous solution, it was found that the folding of the polymer chains can be strongly influenced by the type of salt and this ability follows a trend called the Hofmeister series. While this effect is well known in solution, the influence on the swelling behavior of PNIPMAM thin films has yet to be investigated thoroughly. We aim to elucidate the underlying mechanism by spectral reflectance and time-of-flight neutron reflectometry on a macroscopic scale and by in situ Fourier-transform infrared spectroscopy on a molecular level.

Primary authors: CUBITT, Robert; GEIGER, Christina (Technical University of Munich, Chair of Functional Materials); HILDEBRANDT, Viet; KREUZER, Lucas P. (TUM Physik E13); Prof. LASCHEWSKY, André; MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie); REITENBACH, Julija; WANG, Peixi (Workgroup Polymer Interfaces, TUM Department of Physics, Technical University of Munich)

Presenter: REITENBACH, Julija

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **46** Type: **Poster**

Morphology control of Titanium Thin Films in a low temperature process

Tuesday, December 7, 2021 10:30 AM (1h 30m)

A low-temperature routine to realize inorganic amorphous electron-transport layers (ETLs) is of great importance for the commercialization of perovskite solar cells. The fabrication of ETLs at low temperature is energy saving and compatible with flexible substrates. In this work, titanium thin films are synthesized at low temperature (below 100 ℃) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-b-polyethylene oxide (PS-b-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). Morphology tailoring of titanium thin films in the low-temperature process is achieved by managing phase separation of the polymer template. The solvent category for the sol-gel solution is varied to tune the thin film morphologies. Scanning electron microscopy is used to study the structure of the titania films.

Primary authors: PAN, Guangjiu (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); LI, Nian (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); YIN, ShanShan (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); GUAN, Tianfu (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); LIANG, Suzhe (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); Prof. MÜLLER-BUSCHBAUM, Peter (1 Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany; 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: PAN, Guangjiu (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **47** Type: **Poster**

Gracing incidence scattering as a method to understand the influence of non-halogenated solvents on the morphology of organic solar cells

Wednesday, December 8, 2021 11:35 AM (25 minutes)

Lately, organic solar cells (OSCs) have gained increasing attention due to their rapidly increas- ing efficiencies as well as the relatively easy scalability in their manufacture. However, their production relies heavily on the use of halogenated solvents, as organic solar cells made with environmentally friendly solvents often suffer from reduced performance, which is associated with the reduced solubility of some OSC materials. This can be partially reversed by raising the temperature of the solvents during formation of the bulk-heterojunction (BHJ), increasing the solubility of the respective material.
We investigate and compare the changes in morphology and performance stability of PTQ10:BTP-4F OSCs processed from various solvents, utilising operando grazing-incidence small and wide angle X-ray scattering during illumination and solar cell operation. We further show the impact of solvent composition on the charge carrier dynamics in the respective BHJs using time-resolved transient absorption spectroscopy, analysing the connection between thin-film morphology and device performance in polymer:non-fullerene acceptor OSCs.

Primary authors: HARTSCHUH, Achim (4Department Chemie und CeNS, Ludwig-Maximilians-Universität München, Munich, Germany); TOTH, David (4Department Chemie und CeNS, Ludwig-Maximilians-Universität München, Munich, Germany); HEGER, Julian; SPANIER, Lukas; IGLEV, Hristo (Lehrstuhl für Laser- und Röntgenphysik, Physik-Department, TU München, Garching, Germany); NUBER, Matthias (TU München); SCHWARTZKOPF, Matthias (DESY); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); HOUSSAINI, Rachid (4Department Chemie und CeNS, Ludwig-Maximilians-Universität München, Munich, Germany); KEINBERGER, Reinhard (Lehrstuhl für Laser- und Röntgenphysik, Physik-Department, TU München, Garching, Germany); GUO, Renjun (Physics E13, Technical University in Munich); ROTH, Stephan (DESY / KTH); ZOU, yuqin

Presenter: SPANIER, Lukas

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **48** Type: **Poster**

Single crystal studies on multiferroic LiFe(WO4)2

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Due to their application potential for new types of memory devices, the research on multiferroic materials has attracted strong interest during the last decades. A prominent mechanism that drives multiferroic behavior is given by the inverse Dzyaloshinskii-Moriya interaction, which yields the shift of a non-magnetic ligand ion due to a non-collinear magnetic structure. It was shown on a powdered sample of $LiFe(WO_4)_2$ that the onset of a spiral spin structure is accompanied by an evolving ferroelectric polarization, whose direction is consistent with the inverse DMI 1. Here, we report on our single crystal investigations on $LiFe(WO_4)_2$, for which we utilized neutron scattering experiments on HEIDI and on KOMPASS [2]. It was possible to determine the magnetic structure of both incommensurate phases at low temperature, which follow the typical sequence of magnetic phases for a type-II multiferroic material. First, in the intermediate phase a spin-density wave forms and subsequently in the multiferroic phase, a chiral spin structure evolves. Furthermore, longitudinal neutron polarization analysis on the cold three-axes spectrometer KOMPASS revealed a partially unbalanced multiferroic domain distribution that develops in the multiferroic phase and even in absence of external fields.
1 Liu et al., Phys. Rev. B 95, 195134 (2017) [2] Biesenkamp et al., Phys. Rev. B 103, 134412 (2021)

Primary author: BIESENKAMP, Sebastian (II. Physikalisches Institut, Universität zu Köln)

Co-authors: GORKOV, Dmitry (FRM2); Dr BRÜNING, Daniel (II. Physikalisches Institut, Universität zu Köln); BERTIN, Alexandre (University Of Cologne); Dr FRÖHLICH, Tobias (II. Physikalisches Institut, Universität zu Köln); Dr FABRÈGES, Xavier (Laboratoire Léon Brillouin); Dr GUKASOV, Arsen (Laboratoire Léon Brillouin); MEVEN, Martin (RWTH Aachen University, Institute of Crystallography - Outstation at MLZ); Prof. BECKER-BOHATÝ, Petra (Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln); Prof. BOHATÝ, Ladislav (Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln); Prof. LORENZ, Thomas (II. Physikalisches Institut, Universität zu Köln); BRADEN, Markus (Universität zu Köln)

Presenter: BIESENKAMP, Sebastian (II. Physikalisches Institut, Universität zu Köln)

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **49** Type: **Talk**

Co-nonsolvency behavior of responsive polymers in thin film/vapor systems

Tuesday, December 7, 2021 4:40 PM (25 minutes)

After exposure to mixed water/cosolvent vapor, hydrated thin films of stimuli-responsive block copolymers with PNIPAM or PNIPMAM blocks exhibit a co-nonsolvency behavior. In a rapid film contraction, in either system, both water and cosolvent are expelled. Film swelling and contraction kinetics from saturated vapor are investigated in time-of-flight neutron reflectometry (ToF-NR) with simultaneous spectral reflectance (SR). Molecular interactions of the solvent with the respective polymer chains are analyzed with Fourier-transform infrared (FTIR) spectroscopy. The response kinetics are found to be dependent on the solvation potential of specific functional groups.

Primary author: GEIGER, Christina (Technical University of Munich, Chair of Functional Materials)

Co-authors: REITENBACH, Julija; WANG, Peixi (Workgroup Polymer Interfaces, TUM Department of Physics, Technical University of Munich); Ms HENSCHEL, Cristiane (Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm, Germany); MANGIAPIA, Gaetano (German Engineering Materials Science Centre (GEMS) am Heinz Maier-Leibnitz Zentrum (MLZ)); MOULIN, Jean-Francois (Hereon); LASCHEWSKY, André; PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: GEIGER, Christina (Technical University of Munich, Chair of Functional Materials)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **50** Type: **Poster**

Operando study of humidity on the performance of perovskite solar cell

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Perovskite solar cells (PSCs) are one of the most promising photovoltaic technologies and reached a certified 25.2% efficiency owing to their tuneable bandgap, high carrier mobility, long diffusion length and so on. The long-term operational stability of PSCs, however, has been not investigated. Herein, we probe the structure change with grazing-incidence small-angle scattering techniques (GISAXS) under high humidity. Also, the solar cell parameters are obtained simultaneously during the device operation. We find that PSCs fabricated with and without caesium iodide (CsI) show differences in the device degradation and morphology change in the perovskite layer. The decrease of open-circuit voltage (VOC) can be attributed to the morphology changes and the evolution of crystallize grain size. With the additive of CsI, solar cells show slow decay of VOC, which is correlated to improved morphology of active layer and passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology change combined with solar cell parameters during the device operation.

Primary author: Mr SUN, Kun

Co-authors: Mr HEGER, Julian; SCHEEL, Manuel (TUM E13); SPANIER, Lukas; JIANG, Xinyu (Technische Universität München Fakultät für Physik); Dr BERNSTORFF, Sigrid (Elettra-Sincrontrone Trieste); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: Mr SUN, Kun

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **51** Type: **Talk**

Heat Transport in Quantum Materials - The Intriguing Phonon Physics in Ever Surprising SrTiO3

Tuesday, December 7, 2021 4:15 PM (25 minutes)

The model perovskite $SrTiO_3$ is well-known for its strongly anharmonic phonon properties underlying the intriguing physics of soft phonon modes. A plethora of unusual thermal transport properties derive from the interplay of ferroelectricity, phonon softening, quantum fluctuations and topological properties, including Poiseuille flow of phonons and the elusive coupling of phonons in $SrTiO_3$ to magnetic fields. We gain new insights by establishing a link between the macroscopic specific heat c_p of $SrTiO_3$ signalizing the displacive structural phase transition, and the soft-phonon behavior in the R-corner of the Brillouin zone. We devise a c_p model which is situated intermediate between the oversimplified Debye model, lacking the strongly temperature-dependent renormalization of phonon frequencies, on the one hand, and computationally expensive first-principles calculations based on self-consistent phonon theory, on the other hand. Most notably, our model replicates the temperature evolution of the specific-heat anomaly close to the cubic-to-tetragonal structural phase transition at T_C ~ 105 K. We demonstrate that the entropy-derived critical exponents are compatible with the Heisenberg universality class in the tetragonal phase, as is expected, and, interestingly, also mean-field Landau behavior in the cubic phase. Our analysis identifies the R-point soft phonons to be simultaneously responsible for both, the specific-heat anomaly close to T_C and a sizeable amount of specific heat in the temperature range below ~10 K. Consequently, the correlation between changes in the phase transition and the Debye temperature can be traced back to be microscopically rooted in the soft phonon physics. Quartic anharmonicity by itself is not sufficient to transform the discontinuous specific heat singularity of an idealized impurity-free compound into the experimentally observed specific-heat anomaly with its quasi-continuous shape. Instead, oxygen vacancies or impurity ions are identified to be responsible for changes of the temperature evolution of the R-corner phonon frequencies.

Primary author: HABICHT, Klaus (Helmholtz-zentrum Berlin für Materialien und Energie)

Co-authors: FRITSCH, Katharina (Helmholtz-Zentrum Berlin für Materialien und Energie); KELLER, Thomas (MPI for Solid State Research, Stuttgart); Dr KOJDA, Danny (Helmholtz-Zentrum Berlin); Dr HOFMANN, Tommy (Helmholtz-Zentrum Berlin)

Presenter: HABICHT, Klaus (Helmholtz-zentrum Berlin für Materialien und Energie)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **52** Type: **Talk**

Poly(N-isopropylacrylamide) Mesoglobules under Pressure

Tuesday, December 7, 2021 5:05 PM (25 minutes)

Upon heating through the cloud point, poly(N-isopropylacrylamide) (PNIPAM) in aqueous solution forms long-lived dispersions of mesoglobules. At atmospheric pressure, these mesoglobules are small and strongly dehydrated, and their further growth and coalescence are hindered by the viscoelastic effect. On the contrary, at high pressures, large, water-rich aggregates are formed by PNIPAM 1. Here, we investigate the transition between these two states by varying pressure in the two-phase state. The size and water content of the mesoglobules and the aggregates are characterized using very small angle neutron scattering (VSANS) at KWS-3, MLZ. As pressure is increased, the size of the mesoglobules increases abruptly, and they take up water. These changes occur at critical pressures, that depend on temperature. Upon decreasing pressure, not all large aggregates transform back into smaller mesoglobules, possibly due to entanglements, which demonstrates the importance of the pathway. The results are of importance for the preparation of polymer nanoparticles by nanoprecipitation.
1 B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017).

Primary authors: NIEBUUR, Bart-Jan (TU München, Physik weicher Materie); PIPICH, Vitaliy; APPAVOU, Marie-Sousai (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH); SCHULTE, Alfons (University of Central Florida); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie)

Presenter: PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **53** Type: **Poster**

The In-Situ GIWAXS Heuristic Tool for Efficient Reduction of High-Quality Big Data

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Large-scale facilities have gained importance for extended characterization methods in the field of material sciences. In particular, structure analysis by highly brilliant X-ray beams is an ideal technique to investigate drying, crystallization, or degradation processes in-situ. These processes require a high time resolution to capture the reaction dynamics, while developments in detector resolution increase the amount of data that must be processed, ideally in real-time. This has raised the necessity to advance data-processing software tools to help the scientist extracting the essential conclusions from big data sets quickly and efficiently.

In this work, we present a self-contained, python-based tool for the analysis of in-situ grazing-incidence wide-angle X-ray scattering (GIWAXS). The focus lies on the performant and loss-free processing of GIWAXS datasets with high system compatibility for the users. In our software, the IN SItu Giwaxs Heuristic Tool (INSIGHT), we included geometrical transformation and corrections similar to GIXSGUI 1 but extended the functionality to arbitrarily positioned and oriented detectors while maintaining full access to the raw data. This allows for post-processing the original data in q-space without any quality loss.
We apply our tool to an exemplary set of in-situ GIWAXS data following the annealing and crystallization process of a thin film of methylammonium lead iodide based perovskite for the application in solar cells.

1 “GIXSGUI: a MATLAB toolbox for grazing-incidence X-ray scattering data visualization and reduction, and indexing of buried three-dimensional periodic nanostructured films,” Z. Jiang, J. Appl. Cryst. 48, pp 917-926 (2015).

Primary authors: REB, Lennart (TUM E13); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Co-authors: SCHEEL, Manuel (TUM E13); SCHWARTZKOPF, Matthias (DESY); Dr ROSEMANN, Christoph (MiNaXS, PETRA III, Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany); ROTH, Stephan (DESY / KTH)

Presenter: REB, Lennart (TUM E13)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **54** Type: **Talk**

Progress toward creation and study of positron-electron plasma using the NEPOMUC positron source

Tuesday, December 7, 2021 4:15 PM (25 minutes)

A Positron-Electron eXperiment (APEX) aims to produce a magnetically confined, low temperature positron-electron plasma in order to test predictions that such a system with equal mass but oppositely charged species, in contrast to nearly all laboratory and astrophysical plasma, is remarkably stable and exhibits other unique plasma characteristics. The magnetic trap consists of a levitated superconducting coil (a=7.5 cm, I=54 kA-turns) that produces a dipolar magnetic field (maximum field around 1 tesla). To reach plasma conditions at a temperature of kT~ 1 eV, in the confinement volume of V≈10 liters, will require injection of between 10^{10} and 10^{11} positrons (and an equal number of electrons) into the trap (see talks by A. Deller and M. Singer on plans to accumulate positrons from the NEPOMUC beam to create large pulses). In this talk, we present design details1 and construction progress for the levitated dipole trap as well as results of experiments in a prototype trap that uses a supported permanent magnet (0.6 T at the pole surfaces). Positrons are successfully injected into the field of the permanent magnet using a combination of ExB drift, magnetic mirroring, and electrostatic reflection. Injection efficiency is preserved even in the presence of a substantial electron space charge[2], which is encouraging for our first load electrons into the trap before injecting positrons to form the plasma. Plans for installation of the levitated dipole system at the NEPOMUC facility will be presented.
1 M.R. Stoneking, et.al., J. Plasma Phys. **86**, 155860601 (2020).
[2] M. Singer, et al., Phys. Plasmas **28**, 062506 (2021).

Primary author: STONEKING, Matthew (Lawrence University)

Presenter: STONEKING, Matthew (Lawrence University)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **55** Type: **Poster**

Degradation Mechanisms of perovskite solar cells under vacuum and one atmosphere of nitrogen

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Perovskite solar cells have been the subject of several studies aimed at increasing their operational stability, but few have looked at the underlying degradation mechanisms. The influence of the environment on the performance of devices during operation has been neglected in previous studies [4]. Using synchrotron radiation-based operando grazing-incidence X-ray scattering techniques, we study the degradation processes of perovskite solar cells operating in vacuum and a nitrogen environment. We discover that light-induced phase segregation, lattice shrinkage, and morphological deformation occur in vacuum, contrary to earlier findings. Only lattice shrinkage occurs during the operation of solar cells under nitrogen, resulting in improved device stability. A higher energy barrier for lattice distortion and phase segregation is related to the different behaviors. Finally, we discovered that the migration of excessive PbI2 in the perovskite layer to the interface between the perovskite and the hole transport layer degrades device performance in both vacuum and nitrogen.

Primary authors: OECHSLE, Anna-Lena; REB, Lennart (TUM E13); GUO, Renjun (Physics E13, Technical University in Munich); WEINDL, Christian (TUM Physik); SCHEEL, Manuel (TUM E13); LI, Nian (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck--Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); YIN, ShanShan (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); LIANG, Suzhe (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); XIAO, TIANXIAO (Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München); CHEN, Wei (Technische Universität München)

Presenter: GUO, Renjun (Physics E13, Technical University in Munich)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **56** Type: **Poster**

Raman spectroscopy setup at the TOFTOF instrument

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The goal of this project was to include a portable Raman spectrometer into the time-of-flight spectrometer TOFTOF. This setup would allow us to measure neutron and Raman spectra of the sample at the same time, under the same conditions and we would be able to vary the temperature of the sample. As the sample evolves with the change of temperature, so does the Raman spectrum and it is important to take these spectra at the same time and same conditions as the neutron spectrum. The first step of this process is to test the setup in the laboratory conditions. We have managed to install the setup in a laboratory and measure some powder samples at room temperature. We have confirmed that the setup was functional and it can be used with some limitations. The ideas for improving the setup, as well as the challenges will be presented. The materials measured were hydrogen storage materials. Raman spectroscopy, along with neutron spectroscopy is a powerful technique for analyzing the bonding and the intermediate phases that appear in the reactions of these materials.

Primary author: ALIC, Amina (TUM)

Co-authors: Dr WOLF, Marcell (TUM); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: ALIC, Amina (TUM)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **57** Type: **Poster**

Improvement of the thermoelectric properties of PEDOT:PSS films via DMSO addition and DMSO/salt post-treatment resolved from a fundamental view

Wednesday, December 8, 2021 10:30 AM (1h 30m)

The combination of dimethyl sulfoxide (DMSO)-solvent doping and physical-chemical DMSO/salt de-doping in a sequence has been used to improve the thermoelectric (TE) properties of poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS) films. A high power factor of ca.105.2 μW m-1 K-2 has been achieved for the PEDOT:PSS film after post-treatment with 10 % sodium sulfite (Na2SO3) in the DMSO/salt mixture (v/v), outperforming sodium bicarbonate (NaHCO3). The initial DMSO-doping treatment induces a distinct phase separation by facilitating the aggregation of the PEDOT molecules. At the same time, the subsequent DMSO/salt de-doping post-treatment strengthens the selective removal of the surplus non-conductive PSS chains. Substantial alterations in the oxidation level, chain conformations, PEDOT crystallites and their preferential orientation are observed upon treatment on the molecular level. At the mesoscale level, the purification and densification of PEDOT-rich domains enable the realization of inter-grain coupling by the formation of the electronically well-percolated network. Thereby, both electrical conductivity and Seebeck coefficient are optimized.

Primary authors: TU, Suo (Institute of Functional Materials); TIAN, Ting; OECHSLE, Anna-Lena; YIN, ShanShan (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); JIANG, Xinyu (Technische Universität München Fakultät für Physik); CAO, Wei (TU München); LI, Nian (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); SCHEEL, Manuel (TUM E13); REB, Lennart (TUM E13); Mr HOU, Shujin (Physics of Energy Conversion and Storage, Physik-Department, Technische Universität München); Prof. BANDARENKA, Aliaksandr (Physics of Energy Conversion and Storage, Physik-Department, Technische Universität München); SCHWARTZKOPF, Matthias (DESY); ROTH, Stephan (DESY / KTH); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: TU, Suo (Institute of Functional Materials)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **58** Type: **Poster**

Investigation and Tuning of Slot-Die Coated Perovskite Solar Cells Using X-Ray Diffraction

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Perovskite solar cells (PSCs) have attracted increasing attention in research and industry due to their high efficiency, low material cost and simple solution-based fabrication process, which allow the manufacture of thin, flexible photovoltaic modules.
In laboratory devices, the efficiency already exceeds 25% and is comparable with c-Si.1 However, one of the most important steps towards commercialisation is upscaling the production of PSCs to a larger area. Slot-die coating is one of the most promising technology being a fast process with minimum material consumption and waste.[2]

Furthermore, the highly tuneable perovskite ink composition strongly determines the final morphology of the film, providing an outstanding opportunity to develop a comprehensive understanding of the kinetic processes during film formation. The focus of the work is the effect of additives, such as methylammonium chloride (CH_3NH_3Cl) and methylammonium bromide (CH_3NH_3Br), on the perovskite layer. A complete study - using spectroscopic and X-ray scattering methods - allowed us to effectively understand the role of the halide atoms in the crystallization process.

The ultimate goal of our work is to investigate suitable ink compositions and the resulting final perovskite thin-film to develop a systematic and reproducible printing technique for printed flexible and high-efficiency PSCs.

Primary author: Mr VITALONI , Andrea (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany)

Co-authors: REB, Lennart (TUM E13); SCHEEL, Manuel (TUM E13); GUO, Renjun (Physics E13, Technical University in Munich); HEGER, Julian; SCHWARTZKOPF, Matthias (DESY); ROTH, Stephan (DESY / KTH); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: Mr VITALONI , Andrea (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **59** Type: **Poster**

The Role of CsBr in Crystal Orientation and Optoelectronic Properties of MAPbI3-based devices

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Yuqin Zoua, Shuai Yuanb, Ali Buyrukc, Johanna Eichhornd, Shanshan Yina, Manual A. Scheela, Tianxiao Xiaoa, Shambhavi Pratapa, Suzhe Lianga, Wei Chena, Christian L. Weindla, Cheng Mub, Ian Sharpd, Tayebeh Americ,&, Matthias Schwartzkopfe, Stephan V. Rothe, f, Peter Müller-Buschbaum*a, g

aLehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany. E-mail: muellerb@ph.tum.de

bDepartment of Chemistry, Renmin University of China, No. 59 Zhongguancun Street, Beijing 100872, P. R. China

cDepartment of Chemistry, Chair of Physical Chemistry and Center for NanoScience (CeNS), University of Munich (LMU), Butenandtstr. 5-13 (E), 81377 München, Germany

dWalter Schottky Institute and Physics Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

eDeutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg, Germany

fKTH, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

gHeinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Orientations of crystal planes impact on the behavior of photogenerated charge carriers and are vital for developing electronic properties of the corresponding devices. Herein, we propose a facile approach to reveal the effect of crystal stacking on the charge carrier kinetics by doping CsBr to enable the formation of a mix-cations perovskite phase. We use grazing-incidence wide-angle X-ray scattering to probe the crystal structure and crystal orientation of the mixed perovskite thin films revealing the effect of the extrinsic CsBr doping on the stacking of the crystal planes. TPV, TPC and tDOS are also used to detect the recombination of the photo-generated charge carriers and the trap-state density. It is demonstrated that CsBr compositional engineering can effectively tune the crystallization orientation of crystal planes, reduce trap-state density and facilitate photocarriers transport across the absorber and pertaining interface simultaneously. This strategy provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

Primary authors: WEINDL, Christian (TUM Physik); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); SCHWARTZKOPF, Matthias (DESY); PRATAP, Shambhavi (Technische Universität München); YIN, ShanShan (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); ROTH, Stephan (DESY / KTH); LIANG, Suzhe (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany); XIAO, TIANXIAO (Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München); ZOU, yuqin

Presenter: ZOU, yuqin

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **60** Type: **Poster**

Interaction of colloids inks with nanoporous cellulose templates

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Layer formation and annealing of nanoparticles especially colloidal inks applied to porous materials is very relevant for functional coatings and printing. The goal is to distinguish and quantify the differences in structure formation during annealing of deposited colloidal inks on a porous and a solid material. Therefore, we compare two different substrates: As porous template we use a layer of cellulose nano fibers (CNF) – so-called nanopaper – and as non-porous reference medium silicon. We use novel colloidal inks consisting of poly-butylmethacrylate (PBMA) and poly-sobrerolmethacrylate (PSobMA) in aqueous solution. We studied the deposition and the subsequent structural and morphological changes during annealing of the colloidal layers in real-time. We use grazing incidence small-angle neutron scattering (GISANS) and grazing incidence small-angle X-ray scattering (GISAXS). During deposition part of the liquid enters the CNF layer while part of the solvent and the colloids remain on top of the nanopaper surface, leading to a complex drying process. Our results show that the CNF- and colloidal layer will change if the glass transition temperature of the colloids is exceeded.

Primary author: HARDER, Constantin (DESY & TUM)

Co-authors: Mrs BETKER, Marie (DESY & KTH); Mr ALEXAKIS, Alexandros (KTH); BRETT, Calvin (KTH & DESY); Mrs ELISABETH, Erbes (DESY & Uni Göttingen); VAGIAS, Apostolos (FRM2 / TUM); Mr CHUMAKOV, Andrei (DESY); GENSCH, Marc; Dr QING, Chen (DESY); SOCHOR, Benedikt (University Würzburg); Dr SCHWARTZKOPF, Matthias (DESY); Mr RUBECK, Jan (DESY); KREUZER, Lucas (MLZ (FRM II, TUM)); WIDMANN, Tobias (TU München, Physik Department, LS Funktionelle Materialien); PORCAR, Lionel (ILL); Dr VOROBIEV, Alexei (ILL); Dr ROGERS, Sarah (ISIS); Prof. MANSSON, Martin (KTH); Mr SÖDERBERG, Daniel (KTH); Prof. MALMSTRÖM, EVA (KTH); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); ROTH, Stephan (DESY / KTH)

Presenter: HARDER, Constantin (DESY & TUM)

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **61** Type: **Poster**

Morphology control of PS-b-P4VP templated monolayer mesoporous Fe2O3 thin films

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Mesoporous Fe2O3 thin films with large area homogeneity demonstrate tremendous application potential in photovoltaic industry, lithium ion batteries, gas or magnetic sensors. In the present work, the synthesis of morphology-controlled Fe2O3 thin films is realized with the polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) diblock copolymer assisted sol-gel chemistry. The effect of the solvent category and polymer-to-FeCl3 ratio is systematically investigated during the sol-gel synthesis process. Spin coating is used for the thin film deposition and a calcination process in the air condition is used for removing the PS-b-P4VP polymer template. For both DMF and 1,4-dioxane solvent system, nanosluster structures are obtained with low PS-b-P4VP concentration, which is supposed to be the result of the weak phase separation property and thereby the weak template effect of the block polymer. When the concentration of the PS-b-P4VP reaches the critical point of micellization, spherical and wormlike porous structures can be specifically formed in the DMF and 1,4-dioxane solvent system, respectively. The further increase of the polymer-to-FeCl3 ratio leads to the enlargement of the spherical pore size in the DMF system and the shrink of center-to-center distance of the worm like structure in the 1,4-dioxane system. Moreover, DMF/1,4-dioxane solvent mixture with different volume ratios are applied for the sol-gel solution preparation to trace the effect of the solvent selectivity on the thin film morphology. By adjusting the preferential affinity of the solvent mixture to the polymer blocks, a spherical to wormlike pore shape transition is observed near a critical ⊠⊠ value of 0.77.

Primary authors: Mr WEINDL, Christian L.; Dr SCHWARTZKOPF, Matthias; Ms LI, Nian; YIN, Shanshan; Ms ROTH, Stephan V.; Mr CAO, wei

Presenter: YIN, Shanshan

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **62** Type: **Poster**

Hardening phase precipitation study in the new VDM® Alloy 780 by in-situ high temperature neutron scattering techniques

Tuesday, December 7, 2021 10:30 AM (1h 30m)

In order to improve the microstructure and mechanical properties of newly developed Ni-base superalloy VDM® Alloy 780 it is necessary to understand the γ' hardening phase precipitation process. Here the precipitation process was studied in-situ by time-of-flight (TOF) neutron diffraction (ND) and small-angle neutron scattering (SANS) experiments at high temperature, which allowed us to characterize the obtained γ' precipitates, amount and sizes (by SANS from the very early stages) and the misfit between matrix and precipitates (by ND). Besides, atom probe tomography (APT) and scanning electron microscope (SEM) provided further details on microstructural and chemical composition.

The precipitation of γ' phase at 720 ℃ and its size and volume fraction changes as a function of time was monitored in two differently solution-annealed samples. It appears that the obtained results depend on the heat treatment history of the sample. Two particle size distributions of γ' precipitates were detected by SANS after 2 h in the case of the sample with an extra step after solution-annealing. Variation in heating rates of SANS and TOF ND measurements results in different precipitates nucleation and growth kinetics. A final heat treatment at 620 ℃ does not lead to a similar precipitation or growth process.

The in-situ SANS measurements at 750 ℃ of the fully precipitation hardened sample with two particle size distributions of γ' precipitates at RT confirms the matrix-diffusion-controlled Ostwald ripening of the precipitates.

Primary authors: KIRCHMAYER, Andreas (Department of Materials Science & Engineering, FAU Erlangen-Nürnberg); SOLIS, Cecilia; KÜMMEL, Frank (MLZ TUM); Dr DA SILVA, Ivan (SIS Facility, Science and Technology Facilities Council (STFC)); HAFEZ, Masood (VDM Metals International GmbH); BERAN, Premysl (Nuclear Physics Institute CAS); GILLES, Ralph; MUEHLBAUER, Sebastian; NEUMEIER, Steffen (Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg)

Presenter: SOLIS, Cecilia

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **63** Type: **Poster**

Investigating the HiPIMS deposition of gold onto polymers

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Gold deposition via high power impuls magnetron sputtering (HiPIMS) allows to coat thin metal layers on heat sensitive materials allowing increased adhesion compared to an evaporated gold layer. In addition, this particular technique allows deposition at a lower deposited thermal energy. However, the low temperature nucleation and growth processes of HiPIMS are not sufficiently known. Therefore, we investigate the morphology and structure of thin gold layers on three polymers, namely Polystyrene (PS), Polyvinylalcohol (PVA) and Polyvinyl-4-pyridin (PV4P). The polymers are spincoated onto silicon to obtain ~ 40 nm polymer thin films as substrates. These polymers are of interest as they show different functional moieties and thus are expected to influence the growth of the gold layer. We present first results of our investigations using atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing incidence small angle X-ray scattering (GISAXS).

Primary author: BULUT, Yusuf

Co-authors: DREWES, Jonas (LS Materialverbunde, Institut für Materialwissenschaft, CAU); FRAUPEL, Franz (Kiel University); RIECK, Kristian (Kiel University); SCHWARTZKOPF, Matthias (DESY); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); ROTH, Stephan V.; STRUNSKUS, Thomas (Kiel University)

Presenter: BULUT, Yusuf

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **64** Type: **Poster**

Water Dynamics in Aqueous Poly(N-isopropylacrylamide) Solutions with a Methanol Cosolvent

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Cooperative dehydration is a major driving force for the demixing transition in poly(N-isopropylacrylamide) (PNIPAM), causing the polymer chains to collapse at the cloud point, followed by aggregation in aqueous solution. The motion of the hydration water is slowed down compared to bulk water and it is crucial in the solvation behavior in the presence of a co-solvent such as methanol. QENS measurements were conducted on PNIPAM in a 80% H2O / 20% methanol mixture at variable temperature and pressure with the time-of-flight spectrometer TOFTOF 1. Hydration water is partially released at the demixing transition. The release and adsorption of solvent by the polymer chains correlate with a change in effective solvent composition as evidenced by the diffusive properties of bulk water. At high pressure the solvent phase is enriched with methanol near the cloud point implying that water is preferentially adsorbed.
1 B.-J. Niebuur et al., Macromolecules 54, 4387 (2021)

Primary authors: NIEBUUR, Bart-Jan (TUM Physik-Department E13); LOHSTROH, Wiebke; KO, Chia-Hsin (E13, Physik-Department, Technische Universität München.); APPAVOU, Marie-Sousai (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH); SCHULTE, Alfons (University of Central Florida); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie)

Presenter: SCHULTE, Alfons (University of Central Florida)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **65** Type: **Talk**

Measurement of the Pseudmagnetic precession of polarized 3He

Tuesday, December 7, 2021 1:40 PM (25 minutes)

The pseudomagnetic precession of neutrons in polarized nuclei is caused by the incoherent neutron scattering cross section and leads to a real spin rotation of polarized neutrons. This precession however does not come from "magnetic fields" but directly from scattering at the nucleus. The pseudomagnetic precession of 3He is itself of high for few-body nuclear effective field theories to test nuclear flied models and to understand neutron scattering from quantum liquids. Novel neutron optics using polarized media for "pseudomagnetic neutron prisms" and could be the focus of future studies. However, the two main experimental results for the incoherent scattering cross section of 3He at the ILL and NIST disagree by bout 2 sigma. As a "calibration" for experiments with polarized 129Xe and 131Xe we briefly measured the 3He cross section a recent experiment. Our result, while having very low statistical error, gave a value several sigma (of the statistical error) below the other published results. Consequently, more work is justified. Given the on-site resources for 3He polarization at the JCNS, the JNSE is ideal to attempt to resolve the discrepancy between the published 3He results. Even at a reduced cold neutron flux of the FRM2 without its cold source, viable experiments can indeed be conducted as we measure the direct beam. This would make a topic of good scientific interest with good experimental feasibility to conduct within the next years it JNSE.

Primary authors: Dr GOODSON, Boyd (Southern Illinois University); BABCOCK, Earl; Mr LU, Hao (Indiana University); HOLDERER, Olaf; Dr SNOW, William M (University of Indiana)

Presenter: BABCOCK, Earl

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **66** Type: **Poster**

A search for Parity Violation in Neutron Transmission through Polarized 139La

Tuesday, December 7, 2021 10:30 AM (1h 30m)

We propose to measure a parity-odd asymmetry A in the forward scattering amplitude for neutrons on the p-wave resonance in 139La at 0.73 eV from the correlation k•I, where k is the neutron momentum and I is the spin of the nucleus. One motivation is to take another step towards a future time reversal (T) violation experiment in polarized neutron transmission through polarized 139La 1. The search for new sources of time reversal (T) violation is one of the highest intellectual priorities in nuclear/particle/astrophysics. Our long-term plan is to investigate T violation in neutron interactions with heavy nuclei by searching for a parity (P)-odd and T-odd component in the neutron forward scattering amplitude using polarized neutrons and polarized 139La nuclei from some new interaction beyond the Standard Model of particles and interactions. It is important to measure this k•I correlation, which is an important source of systematic error. Second, this measurement can also fix the key spectroscopic parameter that determines the sensitivity of the T violation search, which depends on the fractions ΓpI±1/2/(ΓpI-1/2+ΓpI+1/2) of the total width of the 0.73 eV resonance in the I±1/2 channels [2]. A previous measurement by Alfimenkov et al [3] of A=0.31±0.09 is not accurate enough for this purpose. If we confirm the size of A implied by this previous work, it would represent the largest amplification of a symmetry-violating amplitude in nuclear/particle physics and therefore a scientific result of general interest.

1 P. Fadeev and V. V. Flambaum, Physical Review C 100, 015504 (2019), [2] V. P. Gudkov and H. M. Shimizu, Physical Review C 97, 065502 (2018), [3] V. P. Alfimenkov et al, Physics of Atomic Nuclei 59, 1861 (1996), [4] T. Okudaira et al, Physical Review C 97, 034622 (2018).

Primary authors: BABCOCK, Earl; SNOW, William M (University of Indiana); ET, AL. (NOPTREX COLLABORATION)

Presenter: SNOW, William M (University of Indiana)

Session Classification: Poster Session

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **67** Type: **Poster**

Self-compensated Neutron Super Mirror Magnetic Yoke to Reduce Stray Fields

Wednesday, December 8, 2021 10:30 AM (1h 30m)

supper mirror(SM) arrays to greatly reduce stray magnetic fields by using self compensation. This yoke is a minor modification to the typical existing magnetic yokes used for polarized SM arrays, often consisting of rows of very strong permanent magnets, such as NbFeB, arranged on either side between a cavity made of a pair of thick (> 1 cm) soft iron plates. Such configurations can produce high fields (on the order of 500 G) over the large volume of the SM array, however they also create an external dipole field. One can passively shield such devices with additional magnetic layers or shells of μ-metal, soft iron, or even steel, but this adds extra weight, complexity and size while not completely trapping the stray magnetic flux. Therefore we developed and produced a modification to the existing magnetic yoke to compensate the stray fields at long range. This is done by adding a balanced amount of magnets with opposite magnetization to the original yoke, thus effectively canceling the stray field at distances of relevance to neutron instrumentation. The final device is similar to a simplified cladded magnet structure, and can be produced essentially as a bolt-on addition to existing polarized SM array magnetic yokes. This modification, in addition to eliminating the stray dipole fields at long range, actually increases the magnetic field inside the active area of the yoke.

Primary authors: GORKOV, Dmitry (FRM2); BABCOCK, Earl; BRADEN, Markus (Universität zu Köln); MONKENBUSCH, Michael (FZF, JCNS-1); HOLDERER, Olaf; BOENI, Peter; MATTAUCH, Stefan (FZ-Juelich); PASINI, Stefano (Forschungszentrum Juelich GmbH)

Presenter: BABCOCK, Earl

Session Classification: Poster Session II

Track Classification: Neutron Methods

Contribution ID: **68** Type: **Poster**

Tunable spin-flop transition in artificial ferrimagnets

Tuesday, December 7, 2021 10:30 AM (1h 30m)

In the present work authors studied magnetic and structural properties of Fe/Pd/Gd superlattices. The particular system [Fe(35 Å)/Pd(t)/Gd(50 Å)/Pd(t)]x12 was chosen with different layer thicknesses of Pd spacer.
By means of x-ray low-angle diffraction (reflectometry, XRR) and scanning transmission electron microscopy (STEM) with the energy dispersive x-ray (EDX) microanalysis the structural quality of the superlattices was attested.
SQUID and PNR techniques were used to analyze the magnetic properties.

It was shown that the insertion of a thin (t=10–14 Å) Pd layer between Fe(35 Å) and Gd(50 Å) layers into multilayer structure allows a considerable reduction the spin-flop transition field.

Study of the structure indicates that in the specified range of thicknesses, Gd and Pd are intermixed into a homogeneous alloy.

By measuring neutron spin-flip scattering we have detected the presence of a magnetically non-collinear state at temperatures T < 50 K in magnetic fields of above H > 500 Oe for the samples with 10 Å - t - 14 Å. By using an extended Stoner-Wohlfarth model we were able to describe the observed transition as a competition of Zeeman energy, bilinear interaction of order of 1 erg/cm2, and biquadratic addition of the order of 0.5 erg/cm2. The coupling energies can be tuned by varying the thickness of the spacer between

Primary authors: KRAVTSOV, Evgeny; ANTROPOV, Nikolay; MAKAROVA, Marina; KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research)

Presenter: ANTROPOV, Nikolay

Session Classification: Poster Session

Track Classification: Quantum Phenomena

Contribution ID: **69** Type: **Talk**

Study of point defects in group-III nitrides by means of positron annihilation spectroscopy

Tuesday, December 7, 2021 9:05 AM (25 minutes)

Gallium nitride (GaN) and related alloys [(AlGaIn)N] are promising materials for next generation power electronics. For GaN, for example, because of its wide bandgap, high saturation electron velocity, sufficient thermal conductivity, and high breakdown voltage, it yields a higher figure of merit compared with that of other semiconductors for power devices such as Si and SiC. The presence of point defects with high concentration, however, are the major obstacle to fabricate (AlGaIn)N-based devices. Especially, an understanding of the relationship between dopant activation and point defects is one of key topics. Positron annihilation is a powerful technique for characterizing vacancy-type defects in semiconductors. We have used monoenergetic positron beams to probe vacancies in ion-implanted GaN and GaN grown on Si substrate [1—6]. In the presentation, several possibilities of the application of PLEPS to the study of vacancy-type defects in group-III nitrides will be proposed.

1. A. Uedono, T. Tanaka, N. Ito, K. Nakahara, W. Egger, C. Hugenschmidt, S. Ishibashi, and M. Sumiya, Thin Solid Films 639, 78-83 (2017).
2. A. Uedono, S. Takashima, M. Edo, K. Ueno, H. Matsuyama, W. Egger, T. Koschine, C. Hugenschmidt, M. Dickmann, K. Kojima, S. F. Chichibu, and S. Ishibashi, Phys. Stat. Sol. B 255, 1700521(1-9) (2018).
3. A. Uedono, T. Nabatame, W. Egger, T. Koschine, C. Hugenschmidt, M. Dickmann, M. Sumiya, and S. Ishibashi, J. Appl. Phys. 123, 155302(1-8) (2018).
4. A. Uedono, H. Iguchi, T. Narita, K. Kataoka, W. Egger, T. Koschine, C. Hugenschmidt, M. Dickmann, K. Shima, K. Kojima, S. F. Chichibu, and S. Ishibashi, Phys. Stat. Sol. B 256, 1900104(1-12) (2019).
5. A. Uedono, W. Ueno, T. Yamada, T. Hosoi, W. Egger, T. Koschine, C. Hugenschmidt, M. Dickmann, and H. Watanabe, J. Appl. Phys. 127, 054503(1-8) (2020).
6. A. Uedono, K. Shojiki, K. Uesugi, S. F. Chichibu, S. Ishibashi, M. Dickmann, W. Egger, C. Hugenschmidt, and H. Miyake, J. Appl. Phys. 128, 085704(1-8) (2020).

Primary authors: Prof. UEDONO, Akira (University of Tsukuba); HUGENSCHMIDT, Christoph; DICKMANN, Marcel; Dr ISHIBASHI, Shoji (AIST); EGGER, Werner (Universität der Bundeswehr München)

Presenter: Prof. UEDONO, Akira (University of Tsukuba)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **70** Type: **Poster**

Evaluation and comparison of scattering data driven molecular dynamics simulations of water models

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Molecular dynamics simulations are an important tool in evaluating scattering data. They have a high potential, which is even further increasing with the ever increasing computation power and isn't yet fully exploited. For some systems, reliable simulations are already available that are compatible with measured data. For other systems, however, the agreement between simulation and experiment is not satisfactory yet. In this work, we compare measured and simulated data as well as mathematical models on the example of different liquid water models in order to later optimize the underlying forcefields in the simulation as well as the hitherto used mathematical models of the evaluation.
The water molecular dynamics simulations were performed with the program LAMMPS and the program SASSENA was used to calculate the corresponding scattering signals. The outcomes were compared to already existing experimental data and changes in the underlying force fields where evaluated in terms of their impact on the behaviour of the simulation. The long-term aim is to create a new evaluation tool, adapting the parameters of molecular dynamics simulations to match the scattering experiments.

Primary authors: REICH, Veronika (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); MÜLLER, Martin (Helmholtz-Zentrum Geesthacht)

Presenter: REICH, Veronika (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon)

Session Classification: Poster Session II

Track Classification: Neutron Methods

Contribution ID: **71** Type: **Talk**

A buffer-gas trap for the NEPOMUC positron beam

Tuesday, December 7, 2021 4:40 PM (25 minutes)

Buffer-gas traps (BGT) can efficiently accumulate positrons from a continuous source into a dense, low-energy nonneutral plasma. Inelastic collisions between positrons and nitrogen molecules promote capture of the former in the electric potential minimum created by a series of cylindrical electrodes in a uniform magnetic field. Usually, the positron source is a neon-moderated radioisotope of sodium. Here, we describe our plans to install a BGT at the NEPOMUC positron facility. Neutron-induced pair production and tungsten remoderation deliver a mono-energetic beam of $\sim 10^8$~e^+/s (i.e., ten times more intense than a typical moderated β^+ beam). The BGT will accumulate hundreds of millions of positrons from the NEPOMUC beam every 30~s. Together with a high-field multi-cell trap, the BGT will be a crucial component of the APEX low-energy electron-positron pair plasma experiment. The trap-based pulsed positron beam will extend the capabilities of the NEPOMUC and will facilitate a range of new applications, including (almost) background-free positron-annihilation-induced Auger-electron spectroscopy.

Primary author: DELLER, Adam (IPP)

Presenter: DELLER, Adam (IPP)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **72** Type: **Poster**

A capillary battery cell setup for in-operando x-ray investigation of solid polymer electrolytes

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Lithium-Ion Batteries turned out as an indispensable energy supplier in modern society which however suffers from safety concerns due to the flammability of the liquid electrolyte. Solid polymer electrolytes (SPEs) can bypass this obstacle and therefore represent a serious alternative to conventional electrolytes. Especially single-ion conducting polymers (SICPs), which have the anion covalently bonded to the backbone of the polymer and thus exhibit a theoretical transference number of unity, are of great interest in battery research. This property is especially interesting for lithium metal batteries due to the ability of supressing dendritic growth. In addition to that, these polymers show reasonable high ionic conductivities, what makes commercialization possible. Here, the SICP Poly((trifluoromethane)sulfonimide lithium styrene) (PSTFSILi) with Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) is used as SPE and capillary battery cells are fabricated and tested. This special cell type allows the observation of the structural evolution of the polymer electrolyte during cycling of the battery with small/wide angle x-ray scattering (SAXS/WAXS).

Primary authors: APFELBECK, Fabian Alexander Christian (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany); Prof. MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: APFELBECK, Fabian Alexander Christian (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany)

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **73** Type: **Poster**

Q-averaging procedures for neutron diffraction pattern calculation from atomic simulations

Tuesday, December 7, 2021 10:30 AM (1h 30m)

There are various methods for diffraction pattern calculation of powders, differing in Q-averaging procedures. Three of these were studied in detail: (1) The structure factor formula sums up all the hkl planes for a Q-vectors despite their respective orientations. Only peak intensities are calculated and the peak shape is arbitrary. (2) A Monte Carlo (MC) method of averaging used i.a. by the program SASSENA involves a number of random Q-points over which the computed intensity is averaged. (3) The Debye Formula considers only interatomic distances and the integration is taken with respect to scattering angle and the scattering is weighted as the fraction of the Ewald sphere surface area.
The structure factor intensity has to be normalized on the Ewald sphere surface area in order to yield the same result as the Debye formula – with the drawback that the peak shapes are arbitrary. Only a sample of one million Q-points was enough to reproduce the Debye formula for monoatomic powders by the MC method, but still insufficient for biatomic crystals. The time for the monoatomic compound there exceeded an hour (C++) while the Debye calculation is finished on the minutes time scale (python).
Summing up, the Debye formula appears to be the best and the most time-efficient way for crystalline powder diffraction modeling.

Primary authors: KUZNETSOVA, Anastasiia (WPN Hereon Garching branch); MAJUMDAR, Arnab (Helmholtz Zentrum hereon); MÜLLER, Martin (Helmholtz-Zentrum Geesthacht); BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); REICH, Veronika

Presenter: KUZNETSOVA, Anastasiia (WPN Hereon Garching branch)

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **74** Type: **Talk**

MEASUREMENT OF THE SPIN-WAVE STIFFNESS AND THE ENERGY GAP IN THE MAGNON SPECTRUM OF AMORPHOUS FERROMAGNETS BY SMALL-ANGLE SCATTERING OF POLARIZED NEUTRONS

Tuesday, December 7, 2021 5:05 PM (25 minutes)

Amorphous magnetic materials are of considerable interest, both from a fundamental and applied point of view. The low coercive field in an amorphous magnet is an important property for its application as a core material in electrical transformers. The structural and magnetic properties of amorphous magnetic systems can be quite complex. The presence of structural as well as magnetic disorder plays an important role in amorphous systems. However, understanding the formation and growth of spin clusters in amorphous systems is a difficult task, as they properties depend on their morphology under the influence of an external magnetic field. The properties of spin clusters in an amorphous system under the influence of an external magnetic field depend on their morphology. Therefore, from the magnetism point of view, interesting aspects are: (1) correlation between structural and magnetic properties; (2) understanding the behavior of spin clusters and (3) investigation of collective magnetic excitations in such systems.

This work presents studies of magnetic excitations of amorphous ferromagnetic FeNi alloys by small-angle scattering of polarized neutrons. It is widely known that the most direct method of studying magnetic excitations is neutron three-axis or time-of-flight spectroscopy. These methods have a limited range of applicability at small momentum transfer, where magnetic scattering from the amorphous materials is concentrated. Hence, the technique of small-angle scattering of polarized neutrons in inclined geometry was proposed and implemented at the Petersburg Institute of Nuclear Physics in the mid-eighties 1. By measuring the difference in the dependence of scattering intensities at different initial polarization of the neutron beam on the momentum transfer, it is possible to register scattering by spin waves only. In this case, a chiral scattering channel of polarized neutrons results in the asymmetry of the scattering intensity and manifests itself best when an external magnetic field is applied at an angle of 45° [2]. In this case, it turns out that the scattering by spin waves is concentrated in a cone bounded by the cut-off angle θc, that is directly related to the spin wave stiffness. Thus, by obtaining the dependence of the cut-off angle on the applied magnetic field or on the wavelength of neutrons, it is possible to measure the energy gap in the spin wave dispersion.

In this work, we conduct the polarized neutron scattering study on spin waves in amorphous FeNi alloys using the SANS-1 instrument. It is shown that the quadratic spin wave dispersion is gapped: $\varepsilon = Aq^2 + g\mu BH + Eg$. The presence of field independent gap in the spectrum of amorphous ferromagnets has already been previously detected in amorphous microconducts of the compound $Fe_{77.5}Si_{5.5}B_{15}$ [3]. In this report, we will discuss details of the measuring protocol and difficulties encountered in detection of the energy gap using this method.

1 A.I. Okorokov, V.V. Runov, B.P. Toperverg, A.D. Tretyakov, E.I.Maltsev, I.M.Puzeii, V.E.Mikhailova, JETP Lett., 43, 503(1986).

[2] S.V. Grigoriev, E. V. Altynbaev, H. Eckerlebe, A. I. Okorokov, Surface. X-ray, synchrotron and Neutron Investigations, 10, 71-78 (2014).

[3] S. V. Grigoriev, K.A. Pschenichny, I.A.Baraban, V.V. Rodionova, K.A.Chichai, A. Heinemann, JETP Letters, 110, 800 – 806 (2019).

Primary authors: Ms AZAROVA, Liubov (Saint Petersburg State University, 199034 Saint Peters-

burg, Russia); Mr PSCHENICHNIY, Kirill (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of NRC “Kurchatov Institute”, 188300 Gatchina, Russia); HEINEMANN, Andre; Prof. GRIGORIEV, Sergei (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of NRC “Kurchatov Institute”, 188300 Gatchina, Russia)

Presenter: Ms AZAROVA, Liubov (Saint Petersburg State University, 199034 Saint Petersburg, Russia)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **75** Type: **Talk**

Non-collinear long-range coupling in manganates superlattices

Tuesday, December 7, 2021 1:40 PM (25 minutes)

Transition metal oxides display versatile magnetic phenomena that are mediated by various exchange mechanisms thanks to the localized d-electrons Perovskite manganese oxides (manganates) are archetypal examples of such magnetic transition metal oxides. In manganates, the super-exchange and double-exchange interactions play a major role in determining the magnetic phase. The relative strength between the two interactions is tuned by the average number of electrons at Mn sites, which leads to a phase diagram crowded with numerous magnetic phases. In addition, their ideal half-metallicity makes manganates as prominent candidate materials for near future magnetic devices such as magnetic random-access memory (MRAM), and other spin-current applications.
Another property that is invaluable for magnetic devices is the long-range magnetic interaction such as RKKY, which is currently used to generate antiparallel spin configurations in MRAM. Yet, exhaustive investigation of long-range interaction in transition metal oxides have been lacking. There are only few examples where non-collinear magnetic ordering was observed in superlattices composed of different perovskites. Here, we demonstrate that superlattices made of only manganates can exhibit non-collinear magnetic superstructures and present their temperature- and field-dependence using polarized neutron reflectometry. The long-range exchange interaction was tuned by the modulation of dopants using oxide layer-by-layer molecular beam epitaxy, which minimized the detrimental lattice-mismatch between layers. Considering extremely versatile phase diagram of manganates, discovery of non-collinear ordering in our only-manganate superlattices calls for further investigation of manganates superlattices.

Primary authors: KEIMER, Bernhard (Max-Planck-Institut für Festkörperforschung); KIM, Gideok (Center for integrated nanostructure physics); GUASCO, Laura; KELLER, Thomas (MPI for Solid State Research, Stuttgart); KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research)

Presenter: KIM, Gideok (Center for integrated nanostructure physics)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **76** Type: **Poster**

Thin film fabrication in a new laboratory

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Thin film samples for neutron investigation can be fabricated with a Molecular Beam Epitaxy (MBE) setup on site. The MBE setup is part of the additional facilities which can be booked in combination with a neutron instrument proposal at MLZ. Discuss your ideas with the thin film lab staff and then write a proposal. There are two options for access: In remote access the thin film staff fabricates the sample for you and in collaborative access: you fabricate the sample with support by the thin film laboratory staff. First option only works if the growth parameters are well identified.

The MBE setup is equipped with effusion cells, electron guns for electron beam evaporation and a plasma source for use with oxygen or nitrogen. A large variety of deposition materials can be used. Please express your ideas! Compounds may be produced either by codeposition or by shutter modulated growth of individual layers. For in-situ surface structure analysis reflection high and low energy electron diffraction is utilized while Auger electron spectroscopy is applied for in-situ chemical surface analysis.

Recently the MBE setup has been moved into the new laboratory in UYL and a new feature, i. e. the determination of the in situ flux rate of atoms using the principle of atomic absorption spectroscopy is about to be established. This method will enhance the precision in stoichometry drastically.

Thin film samples which are sensitive to ambient conditions are first fabricated in the MBE setup and then measured at the neutron reflectometer MARIA of JCNS utilizing a versatile small ultra high vacuum condition chamber (A. Syed Mohd et al. Rev. Sci. Instrum., 87, (2016) 123909)

In the poster various examples for thin film samples will be presented.

Primary author: PÜTTER, Sabine (Jülich Centre for Neutron Science JCNS, Outstation at MLZ, Forschungszentrum Jülich GmbH)

Presenter: PÜTTER, Sabine (Jülich Centre for Neutron Science JCNS, Outstation at MLZ, Forschungszentrum Jülich GmbH)

Session Classification: Poster Session II

Track Classification: Quantum Phenomena

Contribution ID: **77** Type: **Talk**

Benchmarking autonomous TAS experiments

Tuesday, December 7, 2021 4:40 PM (25 minutes)

With the advancement of artificial intelligence and machine learning methods, autonomous approaches are recognized to have great potential for performing more efficient TAS experiments. In our view, it is crucial for such approaches to provide thorough evidence about respective performance improvements in order to increase acceptance within the community. Therefore, we propose a benchmarking procedure designed as a cost-benefit analysis that is applicable not only to TAS, but also to any scattering method sequentially collecting data during an experiment. For a given approach, the performance assessment is based on how much benefit, given a certain cost budget, it is able to acquire in predefined test cases. Different approaches thus get a chance for comparison and can make their advantages explicit and visible. We specify the key components of the benchmarking procedure for a TAS setting and discuss potential limitations.

Primary author: TEIXEIRA PARENTE, Mario

Co-authors: SCHNEIDEWIND, Astrid; FRANZ, Christian; BRANDL, Georg (Forschungszentrum Jülich); GANEVA, Marina (JCNS at MLZ, Forschungszentrum Jülich GmbH); BOEHM, Martin (Institut Laue-Langevin); Dr NOACK, Marcus (Lawrence Berkeley National Labratory)

Presenter: TEIXEIRA PARENTE, Mario

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **78** Type: **Talk**

LIMPID - Layer-wise Investigation of Measurements on Positron Implantation and Diffusion

Tuesday, December 7, 2021 9:55 AM (25 minutes)

We developed a new analysis tool for positron depth profiles generated by variable energy Doppler-broadening spectroscopy. It allows users to extract positron diffusion lengths by fits to the S parameter measured as a function of implantation energy. The code written in Python is easily accessible and adaptable. In this talk we present the theoretical background of the algorithm implemented, which includes a solution of the time-independent positron diffusion equation. We demonstrate all currently available features and present possible application cases. Furthermore we discuss the performance of the code and compare it to VEPFIT, the current, albeit outdated, standard software.

Primary author: MATHES, Lucian

Presenter: MATHES, Lucian

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **79** Type: **Talk**

Vacuum compatible electronics for positron physics.

Tuesday, December 7, 2021 1:15 PM (25 minutes)

Low-energy positron beams can only be handled inside of high vacuum chambers. As ordinary electronic construction relies on a suite of materials which is not compatible with ultra-high vacuum it is necessary for conventional electronics to be installed on the outside of experimental chambers and beamlines. In this talk we'll showcase our most recent endeavors in overcoming this limitation by developing specialized vacuum-compatible electronic instrumentation and describe how it can be employed to improve low-energy positron experiments.

Primary author: GUATIERI, Francesco (Università degli Studi di Trento)

Co-authors: Mr BRENNER, Kilian (FRM II); ZIMMERMANN, Michael

Presenter: GUATIERI, Francesco (Università degli Studi di Trento)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **80** Type: **Poster**

Magnetic phase diagram of Dy/Co superlattices

Wednesday, December 8, 2021 11:35 AM (25 minutes)

Last years, interest in the Dy/Co system has increased, since it became possible to switch the magnetization of the system without applied magnetic field by means of a femtosecond laser pulses. Important requirements for achieving switchable magnetic films are antiferromagnetic coupling between spins of rare-earth and transition metals and perpendicular magnetic anisotropy (PMA). Therefore, it is crucial to find the correlation between the microstructure of thinner and thicker multilayers and their magnetic properties. The aim of this investigation was to define the influence of Dy thicknesses on the magnetic properties of Dy/Co ultilayers.
A series of [Dy (t Å)/Co (30 Å)]40 (t=4 - 20 Å) multilayers were fabricated by DC magnetron sputtering. Structural characterization of the samples was performed by Magnetic properties were investigated by VSM-magnetometry and polarized neutron reflectometry (PNR) and XMCD.X-ray reflectometry and electron-microscopic studies showed formation of DyCo intermetallic compound and Co nanocrystalline layers during the grown process. Also DyCo intermetallic layers are amorphous. The magnetization DyCo is aligned parallel to normal of sample plane, the Co magnetization is oriented in the direction of applied magnetic field. The superlattices consisting of two layers with uniaxial magnetic anisotropies is considered whose easy axes are oriented perpendicular to each other. By neutron reflectometry we observed strong increase of the intensity of spin-flip scattering which evidences increase of non-collinearity of the system. We found rich phase diagram of Dy/Co heterostructures which arising due to the competition of exchange coupling, magneto crystalline anisotropy and Zeeman energy.

Primary authors: KRAVTSOV, Evgeny; MAKAROVA, Marina; ANTROPOV, Nikolay; KHAYDUKOV, Yury (Max-Planck Institute for Solid State Research)

Presenter: MAKAROVA, Marina

Session Classification: Poster Session II

Track Classification: Quantum Phenomena

Contribution ID: **81** Type: **Talk**

Formation of a micrometer positron beam at the Scanning Positron Microscope

Tuesday, December 7, 2021 2:05 PM (25 minutes)

Positron annihilation lifetime spectroscopy (PALS) is a powerful tool for defect detection and characterization in material science. To investigate inhomogeneous defect distributions, e.g. close to fatigue cracks or dispersive alloy, with PALS a monochromatic pulsed positron beam of variable energy with a diameter in the range of 1 µm and a pulse width of 150 ps FWHM is needed. To this aim the Scanning Positron Microscope (SPM) was developed and built at the Universität der Bundeswehr. To overcome the limit of low count-rates obtainable with laboratory positron sources, the SPM is currently transferred to the intense positron source NEPOMUC at the MLZ in Garching. A sophisticated beam preparation, including multiple remoderation steps, is necessary to reach a lateral resolution in the micro-meter range. An essential component is the RF positron elevator which compensates for the energy loss caused by the remoderation process without altering other important beam properties like time structure and brightness.
In this contribution we will give an overview of the current status of SPM, which has been completely refurbished during the reactor shutdown. To ensure proper operation of SPM at NEPOMUC, stable amplitude, stable frequency and stable phase of the RF-signal are crucial. We report recent developments of the RF positron elevator, in particular a new frequency stabilization system.

Primary author: MITTENEDER, Johannes

Co-authors: DICKMANN, Marcel; EGGER, Werner (Universität der Bundeswehr München); HELM, Ricardo (Universität der Bundeswehr München); DOLLINGER, Günther

Presenter: MITTENEDER, Johannes

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **82** Type: **Poster**

Lithium Diffusion and Ionic Conductivity in Lithium Phosphidotetrelates

Tuesday, December 7, 2021 10:30 AM (1h 30m)

High-performance energy storage solutions are a basic prerequisite for efficient portable devices and the electrification of the transport sector, and by this reaching the CO_2 emission targets. The market and progress demand for advances in electrochemical energy storage and a promising approach towards advanced batteries is the so-called all solid state battery concept, where the liquid electrolyte is replaced by a solid state ion conductor.
In this context, search for new types of lithium-permeating membranes along with detailed investigations of potential solid electrolytes are required. The key target is the understanding of structure-property relationships of solid ion conductors, which is inevitable for a purposeful tailoring of a batch of properties directly relevant for applications.
Material classes such as the family of lithium phosphidotetrelates and -trielates, which contain numerous compounds that combine both a great structural variety and closely related structures, are of particular importance because of their diversity, high lithium conductivity, processability etc.[1−3] Herein, the details of lithium diffusion in a series of structurally related fast ion conducting phosphidotetrelates (e.g., $Li_{14}TtP_6$ and (α-/β-)Li_8TtP_4; Tt = Si, Ge, Sn) are analyzed and compared with respect to the corresponding materials properties. Applying electrochemical impedance spectroscopy and temperature-dependent powder neutron diffraction experiments in combination with the maximum entropy method as well as one-particle potential analysis, enables a thorough study of lithium transport in this class of materials.

1 S. Strangmüller, et al., *J. Am. Chem. Soc.*, **2019**, *141*, 14200-14209.
[2] T. M. F. Restle, et al., *Angew. Chem., Int. Ed.*, **2020**, *59*, 5665-5674.
[3] S. Strangmüller, et al., *J. Mater. Chem. A*, **2021**, *9*, 15254-15268.

Primary author: Dr STRANGMÜLLER, Stefan (Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II))

Co-authors: Dr SENYSHYN, Anatoliy (Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II)); Prof. FÄSSLER , Thomas F. (TUM, Lehrstuhl für anorganische Chemie)

Presenter: Dr STRANGMÜLLER, Stefan (Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II))

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **83** Type: **Poster**

Optimization of printed Perovskite Solar Cells using X-Ray scattering

Wednesday, December 8, 2021 10:30 AM (1h 30m)

In the past few years, perovskite solar cells (PSCs) received a lot of awareness in research due to their low manufacturing cost, high efficiency, and high specific power. For industry, PSCs are very interesting because of their easy solution-based fabrication process and comparable efficiencies with the established c-Si-based solar cells.¹ Thus, the fabrication can be upscaled with low waste deposition technologies like printing. Being fast and using minimal material, slot-die coating is a very promising technique.^[2]
During our work we optimize printed PSCs on flexible substrates and investigate their suitability for the application in space environment.^[3] The objective is the development of PSCs by applying different compositions and measuring techniques like spectroscopy and real-space imaging in combination with X-ray scattering methods.
¹ Green, M., et al. (2021). “Solar cell efficiency tables (version 57)”. Prog. Photovolt. Res. Appl. 29: 3– 15.
^[2] Patidar, R., et al. (2020). “Slot-die coating of perovskite solar cells: An overview.” Materials Today Communications 22: 100808.
^[3] Reb, L., et al. (2020). “Perovskite and organic solar cells on a rocket flight”. Joule 4, 1880–1892.

Primary author: LINDENMEIR, Christoph

Co-authors: VITALONI, Andrea (TUM); REB, Lennart (TUM E13); SCHEEL, Manuel (TUM E13); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: LINDENMEIR, Christoph

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **84** Type: **Talk**

Fissile nuclei rotation effect in 235U(n,γf) process

Tuesday, December 7, 2021 1:15 PM (25 minutes)

T-odd effects in fission of heavy nuclei have been extensively studied during more than a decade in order to study the dynamics of the process. A collaboration of Russian and European institutes discovered the effects in the ternary fission in a series of experiments performed at the ILL reactor (Grenoble) [1-3] and the effects were carefully measured for a number of fissioning nuclei. The analogous effects for gammas and neutrons in fission of 235U and 233U was also measured [3-6] after the observation of T-odd effects for ternary particles accompanying the reaction 235U(n,f) induced by cold polarized neutrons. All experiments up to now were performed with cold polarized neutrons, which suggests a mixture of several spin states of the compound nucleus, the relative contributions of which are not well known. The measurements of gamma and neutron asymmetries in an isolated resonance of uranium is important in order to get "clean" data. Therefore, our team continues to carry out a series of experiments by polarized neutrons with different energies. The present work describes a number of our team's measurements that include the results of T-odd effects in the fission of uranium isotopes by polarized neutrons with different energies at the POLI facility of the FRM II reactor in Garching.

1 P. Jesinger, G.V. Danilyan, A.M. Gagarski, et al., Phys. At. Nucl. 62, 1608 (1999)
[2] P. Jesinger, A. Kotzle, A. Gagarski, et al., Nucl. Instrum. Methods Phys. Res. A 440, 618 (2000)
[3] Y. Kopatch, V. Novitsky, G. Ahmadov et. al., EPJ Web of Conferences 169, 00010 (2018)
[4] G.V. Danilyan, J. Klenke, V.A. Krakhotin, et al., Phys. At. Nucl. 72, 1812 (2009)
[5] G.V. Danilyan, J. Klenke, V.A. Krakhotin, et al., Phys. At. Nucl. 74, 671 (2011)
[6] G.V. Danilyan, J. Klenke, Yu.N. Kopach, et al., Phys. At. Nucl. 77, 677 (2014)

Primary authors: GAGARSKI, Alexei (Petersburg Nuclear Physics Institute of National Research Centre "Kurchatov Institute"); BERIKOV, Daniyar; AHMADOV, Gadir (Joint Institute for Nuclear Research); DANILYAN, Gevorg (Institute for Theoretical and Experimental Physics of National Research Centre "Kurchatov Institute"); DENG, Hao; KLENKE, Jens (FRM II); MASALOVICH, Sergey; NOVITSKY, Vadim (Joint Institute for Nuclear Research); HUTANU, Vladimir; KOPATCH, Yuri (Joint Institute for Nuclear Research)

Presenter: BERIKOV, Daniyar

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **85** Type: **Talk**

Plans for a high field multi-cell trap for positron accumulation

Tuesday, December 7, 2021 5:05 PM (25 minutes)

To form an electron-positron plasma in the 10L volume of a levitated dipole, large numbers of low-energy positrons are needed. The APEX (A Positron Electron eXperiment) collaboration plans to use a combination of multiple Penning-Malmberg traps for the accumulation of such large numbers, which will be installed at the NEPOMUC facility.
In this contribution we introduce the high-field multi-cell trap[1]. The device consists of a master-cell trap and an array of 7 smaller storage cells in the 3 Tesla magnetic field of a superconducting solenoid. It will be used to accumulate pulses of low-energy positrons from the buffer-gas trap and confine them in the storage cells until numbers of $10^{10} - 10^{11}$ positrons are reached. These positrons can be delivered to further experiments, such as the electron-positron plasma experiments as well as to other users of the NEPOMUC facility.
We will present the results of experiments performed at IPP Greifswald[2] with pure electron plasmas of $10^8 - 10^9$ electrons. A particular focus of these experiments was the manipulation of the m=1 diocotron mode because of its importance for the plasma transfer to the off-axis cells. The superconducting magnet will be described, which is used to provide the magnetic field for the multi-cell trap. Several options will be discussed where it could be installed into the beamline. Finally, we will give a preview of the first steps and future experimental program in Garching.
1. C. M. Surko and R. G. Greaves, Radiat. Phys. Chem. 68, 419 (2003)
2. M. Singer et al., RSI (2021) (submitted)

Primary author: SINGER, Martin (IPP)

Co-authors: Prof. STONEKING, Matthew (Lawrence University, Appleton, Wisconsin); Dr DELLER, Adam (IPP Garching); Dr KÖNIG, Stephan (Universität Greifswald); Dr DANIELSON, James (UCSD); Mr STEINBRUNNER, Patrick (IPP Greifswald); Prof. SCHWEIKHARD, Lutz (Universität Greifswald); Prof. SUNN PEDERSEN, Thomas (IPP Greifswald)

Presenter: SINGER, Martin (IPP)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **86** Type: **Talk**

Exploring the synthetic effects on disorder in fast ionic conducting materials using neutron diffraction

Tuesday, December 7, 2021 1:15 PM (25 minutes)

The advent of solid-state batteries has spawned a recent increase in interest in lithium conducting solid electrolytes, especially in the lithium thiophosphates. However, many open questions remain when trying to optimize electrolytes and understand solid state battery chemistries.
In this presentation, we will show how an understanding of the structure-transport properties of the lithium argyrodites Li6PS5X can help tailor the ionic conductivity. We show that an anion site-disorder and anionic charge inhomogeneities are important and that and that tailoring dis disorder leads to improvements of the conductivity.

Primary author: ZEIER, Wolfgang (Justus-Liebig-University Giessen)

Presenter: ZEIER, Wolfgang (Justus-Liebig-University Giessen)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **87** Type: **Talk**

Anion motions in lithium amide-borohydride

Tuesday, December 7, 2021 9:30 AM (25 minutes)

To cover the energy supply with renewable energies is a challenge of local and temporal distribution of renewable sources that requires energy storage technologies. Complex hydrides, which contain ions such as BH4- and NH2-, have a high hydrogen capacity and therefore are candidates for solid state hydrogen storage materials. Many studies reported the improvement of hydrogen reaction in complex hydrides as mixed systems with complex hydrides and/or metal hydrides and by using salt additives.
Li4BH4(NH2)3 contains 11.1 wt.% hydrogen, but it is very stable with the desorption temperature being above 573 K. Nevertheless, in the 6Mg(NH2)2+9LiH+LiBH4 system Li4BH4(NH2)3 is one desorption product, which is liquid under the reaction conditions. As liquid phase beyond solid phases it is supposed to accelerate the mass transport between the reactants and the reaction kinetics. To understand the chemical behaviour and atomic motions of Li4BH4(NH2)3, we measured the anion motions with quasielastic neutron scattering (QENS). We analysed the rotational and long range motions in dependence of temperature and assigned them to BH4- and NH2- using the deuteration technique.

Primary authors: Dr PISTIDDA, Claudio (Helmholtz-Zentrum Hereon); ASLAN, Neslihan (HZG, GEMS at MLZ); MÜLLER, Martin (Helmholtz-Zentrum hereon GmbH); BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); LOHSTROH, Wiebke

Presenter: ASLAN, Neslihan (HZG, GEMS at MLZ)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **88** Type: **Talk**

The Pulsed Low-Energy Positron System PLEPS: Recent Developments

Tuesday, December 7, 2021 1:40 PM (25 minutes)

The Pulsed Low-Energy Positron System PLEPS 1 is a user facility for defect depth-profiling by means of positron lifetime measurements with a monochromatic pulsed positron beam of variable energy ranging from 0.5-21 keV at the intense positron source NEPOMUC at the MLZ in Garching [2].
To further extend the scope of defect characterization of PLEPS various possibilities of in-situ manipulation of the sample during lifetime measurements have been implemented: To drift positrons to layers, interfaces and surfaces it is now possible to apply electrical fields to the sample. A wavelength selective broadband illumination system was installed to manipulate the charge-state of optically active defects. Also, the sample temperature may be varied between 80 K and 600 K. The data-acquisition system was updated to match recent advances at the NEPOMUC remoderator [3]. Moreover, numerical simulations of crucial pulsing components have been conducted to further improve the performance of PLEPS.

1 W. Egger, Proc. Int. School Phys. "E. Fermi", CLXXIV (eds. A. Dupasquier and A. P. Mills jr.), IOS Press: Amsterdam, 419 (2010).
[2] Ch. Hugenschmidt, JLSRF 1 (2015) A 22
[3] M. Dickmann, Acta Phys Pol A 137 (2020) 149

Primary author: HELM, Ricardo (Universität der Bundeswehr München)

Co-authors: EGGER, Werner (Universität der Bundeswehr München); DICKMANN, Marcel; MITTENEDER, Johannes (Universität der Bundeswehr); Dr KÖGEL, Gottfried (Universität der Bundeswehr München); Dr SPERR, Peter (Universität der Bundeswehr München); DOLLINGER, Günther

Presenter: HELM, Ricardo (Universität der Bundeswehr München)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **89** Type: **Poster**

Structure of Molybdenum Nitride Films as Hole-Selective Contacts of Crystal Silicon Solar Cells determined with X-ray Scattering

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Molybdenum Nitride (MoNx) films are investigated as hole-selective layer of crystal Si solar cells due to having a proper work function (5.62 eV) and high conductivity (2000 S/cm). The hole-selectivity so far is limited by the poor surface passivation, which is highly correlated to the interface structure between Si and MoNx. The open circuit voltage and fill factor of devices with thicker MoNx film (200 nm) are better than those of thinner MoNx films (20 nm), which demonstrates that thicker MoNx films induce a better surface passivation and lower contact resistance at the same time. Moreover, the performance is different from MoOx films. Thick MoOx film (>20 nm) will induce a decreased fill factor due to their poor conductivity. In this work, the interface structure change between MoNx and Si is determined with X-ray reflectivity (XRR) analysis to figure out the passivation origin of MoNx films with different thickness. The phase structures and domain size of MoNx films with different thicknesses, compositions and crystallinity are determined with grazing incidence wide and small angle X-ray scattering (GIWAXS and GISAXS) to give important guidance for improving the hole-selectivity of MoNx further.

Primary author: Dr LI, Yajuan (Technical University of Munich)

Co-authors: Mr LI, Yuxiong (Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO), Chinese Academy of Sciences); Dr ZHOU, Jungui (Technical University of Munich); Mr HEGER, Julian Eliah (Technical University of Munich); Mr EVERETT, Christopher Reck (Technical University of Munich); Ms JIANG, Xinyu (Technical University of Munich); Mr GUAN, Tianfu (Technical University of Munich); Prof. JIANG, Chunping (Technical University of Munich); Prof. SUN, Baoquan (soochow university); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: Dr LI, Yajuan (Technical University of Munich)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **90** Type: **Talk**

Dynamics in polymer-fullerene blends for photovoltaic applications, studied with quasielastic neutron scattering

Tuesday, December 7, 2021 9:30 AM (25 minutes)

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed, excitons are created, subsequently dissipated at a material interface and hence free charges are provided. A promising low-bandgap electron donor material is the conjugated polymer PTB7 that is often used in combination with the fullerene derivate PCBM. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, pure PCBM, which acts as electron acceptor, and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching) to determine hydrogen dynamics on a pico- to nanosecond timescale. In addition, two well established techniques for performance enhancement in organic photovoltaics, namely the addition of DIO to the casting solution and a methanol posttreatment of the active layer, are applied and their influence on the polymer dynamics is investigated.

Primary authors: Mr SCHWAIGER, Dominik M. (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); Prof. MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); Dr LOHSTROH, Wiebke (Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: Mr SCHWAIGER, Dominik M. (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **91** Type: **Poster**

Thermal structural stability of lithiated graphites

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Nowadays, 2H graphites are the most common anode materials in LIBs. Despite its overall popularity, the performance of LIBs is still limited by the capability of graphite electrodes to store lithium ions in its structure. Graphite builds up a layered hexagonal structure. During charging and discharging lithium ions are reversibly incorporated in the hexagonal structure resulting in the formation of lithiated graphite phases Li_xC_6 (0 < x < 1) of different kinds.
Despite the overall popularity there is a clear lack of information about the structural behaviour of LixC6 at compositions of x < 0.25 [1, 2]. Even less information is available about the thermal stability of graphite anodes, which becomes more and more popular in the context of all-solid-state-batteries or fast charging.
In the current contribution, a temperature resolved diffraction study on variously lithiated Li_xC_6 samples is presented, where battery graphites were pre-lithiated to a desired lithiation grade in a Li-ion battery and then harvested. The thermal behavior of structural parameters was probed by using powder diffraction studies applying high-energy synchrotron radiation.

1 V. Baran, O. Dolotko, M. J. Mühlbauer, A. Senyshyn, and H. Ehrenberg, J. Electrochem. Soc. 165, 1975-1982 (2018).
[2] A. Senyshyn, O. Dolotko, M. J. Mühlbauer, K. Nikolowski, H. Fuess, and H. Ehrenberg, J. Electrochem. Soc. 160, 3198-3205 (2013).

Primary author: HÖLDERLE, Tobias

Co-authors: MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); SENYSHYN, Anatoliy

Presenter: HÖLDERLE, Tobias

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **92** Type: **Talk**

Tailoring polarized neutron beams by traveling-wave magnetic neutron spin resonance

Tuesday, December 7, 2021 9:05 AM (25 minutes)

We report on experimental tests of the neutron magnetic spin resonator MONOPOL with very cold neutrons. When placed between two supermirror neutron polarizers and operated in a pulsed traveling-wave mode, it allows to decouple time- and wavelength-resolution and can therefore be used simultaneously as electronically tunable monochromator and fast beam chopper. As a first 'real' scientific application we intend its implementation in the PERC facility at FRM II related to high-precision experiments in neutron beta decay.

Primary author: JERICHA, Erwin

Presenter: JERICHA, Erwin

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **93** Type: **Talk**

Time evolution of hydrogen diffusion in Zirconium alloys at 300℃-400℃ by in-situ neutron imaging experiments

Tuesday, December 7, 2021 5:05 PM (25 minutes)

Zr based alloys are widely used in nuclear power plants as nuclear fuel cladding. These materials have an excellent combination of mechanical resistance, corrosion resistance and very low neutron absorption. However, they are susceptible to H degradation, following incorporation of H by a slow oxidation process at operating temperatures (~300℃). For long operational service, Zr based components can fail by a crack growth mechanism associated with the hydrides known as Delayed Hydride Cracking (DHC). H redistributes by solid diffusion and accumulates at stress raisers or cold spots, where it precipitates as a brittle hydride once the solubility is exceeded. Hence, a correct determination of the H diffusion coefficient and the phenomena involved in the dissolution and precipitation of hydrides in Zr alloys are important issues for the safe operation of nuclear power plants. Since the attenuation coefficient for cold neutrons of H is higher than for Zr alloys, neutron imaging represents an excellent technique to study the H concentration and diffusion in Zr alloys. In this work, the time evolution of H diffusion in Zr alloys at temperatures between 300℃ and 400℃ was determined by neutron imaging at the ANTARES cold neutron imaging facility. In-situ annealing was performed, obtaining a spatial resolution of ~30 μm per pixel while the time step analyzed was 15 min. A moving boundary between the regions of the precipitated hydride and the solid solution was observed.

Primary authors: SORIA, Sergio (FRM II); Dr GROSSE, Mirco (KIT); SCHULZ, Michael; SANTISTEBAN, Javier (Centro Atomico Bariloche)

Presenter: SORIA, Sergio (FRM II)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **94** Type: **Poster**

Printed block copolymer templated ZnO photoanodes for photovoltaic applications

Wednesday, December 8, 2021 10:30 AM (1h 30m)

ZnO has received much attention over the past years because it has a wide range of properties, including high transparency, piezoelectricity, wide-bandgap semiconductivity, high electron mobility and low crystallization temperature. To improve the photovoltaic performance of ZnO-based hybrid solar cell devices, an interconnected mesoporous inorganic nanostructure is favorable, which can provide a high surface-to-volume ratio for exciton separation within their lifetime and a good pathway for charge carrier transport. To fabricate the mesoporous inorganic ZnO semiconductors, various methods can be employed, such as chemical vapor deposition, wet chemical method and, hydrothermal synthesis. Among these methods, the diblock copolymer assisted sol-gel synthesis approach has been corroborated by countless reports to be powerful in its morphology tunability.
In the present work, an amphiphilic diblock copolymer is used as the template and suitable printing parameters are selected to fabricate the mesoporous ZnO films with varied morphologies. Grazing-incidence small angle X-ray scattering (GISAXS) is used to probe the inner film morphology without intervening the film formation process or impairing the printed films.

Primary author: TIAN, Ting

Co-authors: YIN, Shanshan; TU, Suo (Institute of Functional Materials); WIENHOLD, Kerstin; MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); WEINDL, Christian (TUM Physik); ROTH, Stephan V.; SCHWARTZKOPF, Matthias (DESY); LIANG, Suzhe (Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany)

Presenter: TIAN, Ting

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **95** Type: **Poster**

Oriented transition dipole moments for high-efficient perovskite light-emitting diodes

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Metal halide perovskite light-emitting diodes (PeLEDs) are regarded as alternative candidates for next-generation display technologies due to their high efficiency, superior color purity and tunable bandgap. However, PeLEDs based on isotropic perovskite emitting layers with randomly oriented emissive transition dipole moments (TDMs) remain to be inefficient to get upper limit efficiencies of planar PeLEDs. In general, horizontal emissive TDMs parallel to the device substrate are suitable for light out-coupling, while emitted light from vertical TDMs is mostly trapped in the device. Therefore, an emissive layer with high ratios of horizontal TDMs is expected to enhance the efficiency of PeLEDs. A high proportion of horizontal TDMs can be obtained by adjusting the thickness and crystal orientation of the perovskite film. Here, we mainly use grazing-incidence wide-angle X-ray scattering (GIWAXS) to study a series of additives, and explore the effect of additives on the crystal orientation of the two-dimensional perovskite films.

Primary authors: Mr ZHOU, Jungui (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, P. R. China; LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Mr CAI, Lei (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, P. R. China); Mr DONG, Xiaohao (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, P. R. China); Mr A. SCHEEL, Manuel (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Ms JIANG, Xinyu (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Dr LI, Yajuan (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, P. R. China; LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Mr SUN, Kun (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Mr HUBER, Linus (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Mr GUAN, Tianfu (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany); Dr SCHWARTZKOPF, Matthias (Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany); Prof. V. ROTH, Stephan (Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany; Department of Fibre and Polymer Technology, KTH, Teknikringen 56-58, SE-100 44 Stockholm, Sweden); Prof. FUNG, Man-Keung (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, P. R. China; Macao Institute of Materials Science and Engineering, Macau University of Science and Technology, Macau, China); Prof. MÜLLER-BUSCHBAUM, Peter (LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany; Heinz Maier-Leibniz Zentrum (MLZ), TU München, Lichtenbergstraße 1, 85748 Garching, Germany)

Presenter: Mr ZHOU, Jungui (Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu

215123, P. R. China; LS Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **96** Type: **Invited talk**

New Insights – How to use neutrons for food and bioprocessing applications

Tuesday, December 7, 2021 1:15 PM (25 minutes)

The preservation of food is one of the most important tasks in food processing. A typical application is lyophilisation or freeze drying and refers to the sublimation of ice to vapour below the triple point. Lyophilisation is employed for dehydrating biopharmaceuticals and high-value foods in frozen state as the structural and nutritional attributes are not affected by the process in contrast to other dehydration techniques. As neutrons are very sensitive for hydrogen molecules, neutron imaging it is a perfect tool to investigate process characteristics.
In this work it is the aim to present an overview of different processes where neutron imaging can be a valuable tool. The focus will be on the freeze-drying experiments, which were carried out at the ANTARES beamline. The results will show the impact of particle size (x1 = 3550 µm and x2 = 70 µm) and solid concentration (c1 = 0.05 w/w and c2 = 0.2 w/w) on drying kinetics and the sublimation front. Also a timeline of different development steps of freeze-drying cells will be shown from the beginning until the current state. At the end an outlook will be given for further planned experiments.

Primary author: GRUBER, Sebastian (TUM)

Co-authors: HILMER, Mathias; Mr THOMIK, Maximilian; VORHAUER-HUGET, Nicole; SCHULZ, Michael; PETERS, Juergen; FOERST, Petra (TUM)

Presenter: GRUBER, Sebastian (TUM)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **97** Type: **Poster**

Novel CDB Data Processing and Evaluation Software

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The Coincidence Doppler-Broadening (CDB) spectrometer at NEPOMUC has recently been upgraded with six additional HPGe Detectors, bringing the total number of detectors to ten. To take full advantage of the even more capable instrument a novel data evaluation software package (STACS) was created.

The software can handle and visualize the data generated by Coincidence Doppler-Broadening Spectroscopy (CDBS) and provides a wide range of tools to analyze such data. Some of the main functions include the extraction of the electron-positron annihilation photo peak from CDB spectra as well as a simple background subtraction algorithm that is able to increase the peak-to-noise ratio of the extracted photo peak further. For the first time it is possible to combine the data from multiple detector pairs, improving measurement statistics. The modular design of the software makes it easy to adapt for future instrument upgrades or even other instruments. Over all the STACS package paired with the upgraded spectrometer is able to perform highly sensitive defect studies or precipitate analysis in solid materials.

Primary author: CHRYSSOS, Leon

Presenter: CHRYSSOS, Leon

Session Classification: Poster Session

Track Classification: Positrons

Contribution ID: **98** Type: **Poster**

In-situ observation of electrode formation in non-fullerene organic solar cells with GISAXS

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Non-fullerene organic solar cells have undergone significant improvements via both, synthesis of novel organic synthesis materials and application of easy fabrication methods. However, device degradtion is still a major problem. For example, the peeling-off of the top electrode fabricated by thermal evaporation leads to an intrinsic device degradation, which is one ofamong the main reasons for the performance losses of organic solar cells. Another disadvantage is the inevitable high temperature during the evaporation process, which can be harmful to the organic materials and is energy extensive thereby prolonging the energy payback times significantly. To overcome these challenges, the magnetron sputtering technique appears very promising for top contact deposition.

For understanding the mechanism of the metal cluster growth on the thin films with various morphologies used in organic solar cells, we use apply in-situ grazing-incidence small-angle X-ray scattering (GISAXS) to observe the morphology changes during the sputter depositioning process. In the present study, the active layer of the organic solar cells is composed of the polymer donor PffDT4T-2OD and the small molecule accepter EH-IDTBR. Both materials were dissolved in 1,2,4-trimethylbenzene and chlorobenzene, respectively to obtain different morphologies of the printed PffDT4T-2OD: EH-IDTBR films. Then 10 nm MoO3 was deposited on their surfaceese films, which acts as the electron blocking layer for thein an inverted solar cell devicegeometry. A 20 nm Al layer is sputtered on top of MoO3 acting as top contact. Notably, the formation of the Al electrode on MoO3 is slower than on the active layer without deposition of MoO3. In addition, SEM and AFM measurements indicate that the morphology impacts the Al growth significantly.

Primary authors: JIANG, Xinyu (Technische Universität München Fakultät für Physik); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); ROTH, Stephan (DESY / KTH); Mr SCHAPER, Simon (TUM); SCHWARTZKOPF, Matthias (DESY)

Presenter: JIANG, Xinyu (Technische Universität München Fakultät für Physik)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **99** Type: **Poster**

Decoding the Self-assembled Plasmonic Nano-structure in Colloidal Quantum Dots for Photodetectors

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Hybrid plasmonic nanostructures have raised great interest for being used in a variety of optoelectronic devices, due to the surface plasmon resonance (SPR). Charge carriers trapped in colloidal quantum dots (QDs) at localized surface defects is a key issue in photodetectors. Self-assembled hybrid metal/quantum dots can couple plasmonics and quantum properties to photodetectors and modify their functionality. Arranged and localized hybrid nanostructures impact on excitons traps and light harvesting. Here, we demonstrate a coupling hybrid structure using self-assembled gold nanoparticles (Au NPs) doped in PbS QDs solid for mapping the interface structures and the motion of excitons. Grazing incidence small angle X-ray scattering (GISAXS) was used to characterize the order of the Au NPs in the hybrid structure. Furthermore, by correlating the sizes of the Au NPs in the hybrid structure with corresponding differences in photodetector performance, we could obtain the interface carriers trapping influences in the coupling structure.

Primary author: GUAN, Tianfu

Presenter: GUAN, Tianfu

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **100** Type: **Poster**

Hybrid Energy Harvester based on Triboelectric Nanogenerator and Solar Cell

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots (QDs) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

Primary authors: XIAO, TIANXIAO (Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München); CHEN, Wei (Technische Universität München); CAO, Wei (TU München); ROTH, Stephan (DESY / KTH); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: XIAO, TIANXIAO (Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **101** Type: **Talk**

Defect studies in tungsten using a slow positron beam

Tuesday, December 7, 2021 9:30 AM (25 minutes)

Predicting helium retention in tungsten is of relevance for future nuclear fusion reactors as it influences tritium uptake and transport, the latter effects being a critical question to achieve tritium self-sufficiency.
While the macroscopic effects of helium agglomeration in tungsten are known it is still an open topic of discussion what the underlying processes on a microscopic scale are. Our goal is to contribute to this discussion by providing experimental results for "simple", i.e only containing vacancy defects, tungsten systems.

We therefore compare samples where defects have been induced by either self-ion bombardment (MeV range), MeV electron bombardment or thermal quenching. While the samples' initial state and post damaging state are also monitored by different types of microscopy, Doppler-broadening spectroscopy is used as the main tool since it shows the highest sensitivity to vacancy-like defects. The positron-annihilation measurements shown have all been performed on a tungsten-moderated, Na-22-based mono-energetic slow positron beam at FRM II which has been modified to deliver acceleration voltages of up to 40 kV.

Primary author: BURWITZ, Vassily Vadimovitch

Co-authors: Ms KÄRCHER, Annemarie (Max-Planck-Intitut für Plasmaphysik); HUGENSCHMIDT, Christoph; Mr ELGETI, Stefan (Max-Planck-Intitut für Plasmaphysik); SCHWARZ-SELINGER, Thomas (Max-Planck-Intitut für Plasmaphysik)

Presenter: BURWITZ, Vassily Vadimovitch

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **102** Type: **Talk**

Focal length tuning in MIEZE Spectroscopy

Tuesday, December 7, 2021 5:05 PM (25 minutes)

The MIEZE technique relies on a fast sinusoidal neutron intensity modulation up to the MHz range, generated by the rotation of the neutron spin in radio-frequency spin flippers, and subsequent conversion to an intensity modulation by a spin analyzer.
This intensity modulation is washed out due to the neutron velocity dispersion.
By carefully choosing the rotation frequencies as well as the distances between sample, detector and spin flippers, a focal point in space is created, the echo point.
Here, the neutron detector is placed. Introducing a field subtraction coil (NSE coil) between the spin flippers, extends the dynamic range of the MIEZE technique towards the low energy resolution end, providing an overlap with conventional spectroscopy techniques. Additionally, the coil can be used to tune the position of the echo point. We will show how the use of a field subtraction coil unlocks the full potential of a MIEZE setup.

Primary authors: JOCHUM, Johanna K.; WENDL, Andreas (Technische Universität München); KELLER, Thomas (MPI for Solid State Research, Stuttgart); FRANZ, Christian

Presenter: JOCHUM, Johanna K.

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **103** Type: **Talk**

On bi-fractal structure of chromatin in rat lymphocyte nuclei

Tuesday, December 7, 2021 1:15 PM (25 minutes)

The small-angle neutron scattering (SANS) on the rat lymphocyte nuclei demonstrates the bi-fractal nature of the chromatin structural organization. The measurements were carried out at the KWS-3 instrument in the momentum transfer range $[10^{-3} - 9 \cdot 10^{-2}]$ nm^{-1} and at the KWS-2 instrument in the momentum transfer range $[9 \cdot 10^{-2} - 2]$ nm^{-1} at MLZ, Garching, Germany.The scattering intensity from rat lymphocyte nuclei is described by power law Q^{-D} with fractal dimension approximately 2.3 on smaller scales and 3 on larger scales. The crossover between two fractal structures is detected at momentum transfer near 10^{-1} nm^{-1}. The use of contrast variation (D_2O-H_2O) in SANS measurements reveals clear similarity in the structural organizations of nucleic acids (NA) and proteins. Both chromatin components shows bi-fractal behavior with logarithmic fractal structure on the large scale and volume fractal with slightly smaller than 2.5 structure on the small scale.
Scattering intensities from chromatin, protein component and NA component demonstrate extremely extensive diapason of logarithmic fractal behavior (from 10^{-3} to approximately 10^{-1} nm^{-1}). We compare the fractal arrangement found in nuclei of the rat lymphocytes with those of the chicken erythrocytes and immortal cell line HeLa. We conclude that bifractal nature of the chromatin arrangement is inherent to nuclei of all these cells. The details of the fractal arrangement - its diapasons and correlation between nuclear acids and proteins are specific for different cells and is related to their functionality.

Primary authors: Dr IASHINA, Ekaterina (Petersburg Nuclear Physics Institute NRC KI); Dr VARFOLOMEEVA, Elena (Petersburg Nuclear Physics Institute NRC KI); Dr PANTINA, Rimma (Petersburg Nuclear Physics Institute NRC KI); Dr BAIRAMUKOV, Viktor (Petersburg Nuclear Physics Institute NRC KI); Mr KOVALEV, Roman (Petersburg Nuclear Physics Institute NRC KI); Ms FEDOROVA, Natalya; PIPICH, Vitaliy; RADULESCU, Aurel (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ); GRIGORIEV, Sergei (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of NRC "Kurchatov Institute", 188300 Gatchina, Russia)

Presenter: Dr IASHINA, Ekaterina (Petersburg Nuclear Physics Institute NRC KI)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **104** Type: **Talk**

Additive manufacturing of custom neutron shielding solutions

Tuesday, December 7, 2021 1:40 PM (25 minutes)

Additive manufacturing using the fused deposition modeling (FDM) allows to easily and inexpensively manufacture complex geometries using 3D printers. Typical base materials are thermoplastics such as polylactic acid (PLA) or acrylonitrile butadiene styrene (ABS). Recently, the availability of 3D printers has increased significantly, enabling the widespread use of additive manufacturing by private users. In science, 3D printing allows to rapidly manufacture prototypes.

An important technical aspect of neutron science is shielding of samples, instrument components and sample environment. Shielding with neutron absorbing material greatly reduces the risk of radiation induced electronic failures during measurements or activation of components. The geometry of the required shielding often pushes the limits of traditional manufacturing techniques.

Therefore, we recently developed a 3D printable shielding material based on PLA in corporation with ColorFabb, allowing to easily manufacture complex shielding geometries. For the shielding material PLA was mixed with boron nitride in hexagonal form, creating an easy to 3D print shielding material, which can be manufactured with most commercial FDM 3D printers.

In this talk we will present the shielding qualities as well as share our experience in working with the shielding material.

Primary authors: NEUWIRTH, Tobias; SEBOLD, Simon (MLZ); SCHULZ, Michael

Presenter: NEUWIRTH, Tobias

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **105** Type: **Talk**

Ultrahigh-resolution neutron spectroscopy of low-energy spin dynamics in UGe2

Tuesday, December 7, 2021 9:30 AM (25 minutes)

Novel electronic phases such as nematic electronic textures or unconventional superconductivity (SC) are frequently observed near zero-temperature magnetic instabilities that arise as a function of a non-thermal control parameter such as pressure. Although it is widely believed that the abundant magnetic fluctuations associated with these quantum phase transitions (QPT) are at the origin of the emergence of novel electronic states, their exact nature remains an outstanding question. Notably, according to theory both the relaxation time and correlation length of the fluctuations are expected to diverge when the quantum critical point is approached. However, to date these divergences have not yet been observed due to the demanding requirements for energy and momentum resolution. Studying the ferromagnetic SC UGe_2 we demonstrate that for ferromagnetic QPTs this problem may be overcome using longitudinal modulation of intensity with zero effort (MIEZE) at the instrument RESEDA. In the case of UGe_2, we reveal purely longitudinal spin fluctuations with a dual nature arising from 5f electrons that are hybridized with the conduction electrons. Local spin fluctuations are perfectly described by the Ising universality class in three dimensions, whereas itinerant spin fluctuations occur over length scales comparable to the superconducting coherence length, showing that MIEZE is able to spectroscopically disentangle the complex low-energy behavior characteristic of quantum materials.

Primary author: HASLBECK, Franz Xaver (Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften)

Co-authors: Dr SÄUBERT, Steffen (Colorado State University); SEIFERT, Marc (Physik Department and Heinz Maier-Leibnitz Zentrum Garching, Technische Universität München); Dr FRANZ, Christian (Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH); Dr SCHULZ, Michael (Heinz Maier-Leibnitz Zentrum Garching, Technische Universität München); Dr HEINEMANN, Andre (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH); Dr KELLER, Thomas (MPI for Solid State Research, Stuttgart); Dr DAS, Pinaki (Los Alamos National Laboratory); Dr THOMPSON, J. D. (Los Alamos National Laboratory); Dr BAUER, E. D. (Los Alamos National Laboratory); Prof. PFLEIDERER, Christian (Physik-Department, Technische Universität München); Prof. JANOSCHEK, Marc (Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institut)

Presenter: HASLBECK, Franz Xaver (Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **106** Type: **Talk**

FM and AFM ordering within a MAX phase bulk

Tuesday, December 7, 2021 2:05 PM (25 minutes)

Neutron diffraction is used to establish room temperature magnetic ordering within a laminar, MAX phase material, for the first time. This finding is the first "building block" within our search for 2D magnetic materials. A coexistence between FM and antiferromagnetic (AFM) ordering is found at 1.5 K, in agreement with previous DFT calculations.

Primary author: RIVIN, Oleg (Nuclear Research Center - Negev (ISRAEL))

Co-authors: Dr GEORGII, Robert (MLZ); Dr CASPI, El'ad (Nuclear Research Center - Negev and Drexel University); Dr HOSER, Andreas (HZB); Dr PESACH, Asaf (NRCN); Mr TAO, Quanzheng (Linkopig University); Prof. BARSOUM, Michel (Drexel University); Prof. ROSEN, Johanna (Linkopig University)

Presenter: RIVIN, Oleg (Nuclear Research Center - Negev (ISRAEL))

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **107** Type: **Talk**

Spectroscopic data and nuclear structure studies using (nth,2γ) reaction and two-step gamma cascade method

Tuesday, December 7, 2021 9:30 AM (25 minutes)

The quality of a number of areas that use nuclear data, such as astrophysical reactions, production of medical isotopes and rare isotope beams, and reactor technology is dependent on the accurate values for gamma ray transitions, level scheme, nuclear level density and radiative strength function. One of the most suitable techniques for the determination of these parameters is the two-step gamma-ray method based on the measurements of the two-step gamma-ray coincidences following thermal neutron capture. This technique can be used to search for new energy levels and gamma transition, place already known gamma transitions in the level scheme, constrain spin values of levels, as well as to determine nuclear level density and radiative strength function.
This technique was most recently successfully applied to 94Nb and 56Mn in experiments conducted at the PGAA facility of Centre for Energy Research (MTA EK), Budapest, Hungary and Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany, respectively. These two experiments combined had, among other results, over 50 new recommendations for energy levels and over 250 new recommendations for gamma transitions. These results proved that this technique can be used to provide new, accurate, data about the level scheme and nuclear structure. Among future plans for usage of this technique is a proposed experiment at the research reactor in Garching, Germany in order to investigate 108Ag and 110Ag nuclei.

Primary authors: KNEŽEVIĆ, David; Dr JOVANČEVIĆ, Nikola (University of Novi Sad, Faculty of Science, Department of Physics, Trg Dositeja Obradovica 3, 21000 Novi Sad, Serbia)

Co-authors: Dr M. SUKHOVOJ, Anatoly (Joint Institute for Nuclear Research, 141980 Moscow region, Dubna, Russia); Dr V. MITSYNA, Liudmila (Joint Institute for Nuclear Research, 141980 Moscow region, Dubna, Russia); Dr DRAGIĆ, Aleksandar (Institute of Physics Belgrade, Pregrevica 118, 11080 Zemun, Serbia); Dr JOKOVIĆ, Dejan (Institute of Physics Belgrade, Pregrevica 118, 11080 Zemun, Serbia); Dr MALETIĆ, Dimitrije (Institute of Physics Belgrade, Pregrevica 118, 11080 Zemun, Serbia); REVAY, Zsolt (PGAA); STIEGHORST, Christian (TUM / FRM II); Ms BLES, Bellona (University of Novi Sad, Faculty of Science, Department of Physics, Trg Dositeja Obradovica 3, 21000 Novi Sad, Serbia)

Presenter: KNEŽEVIĆ, David

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **109** Type: **Poster**

Effects of polymer block length asymmetry and temperature on the nanoscale morphology of thermoresponsive double hydrophilic block copolymers in aqueous solutions

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Nanoscale assemblies in water of novel thermoresponsive and double hydrophilic poly(N-isopropylacrylamide)-block-poly(oligo ethylene glycol methyl ether acrylate) (PNIPAM-b-POEGA) copolymers have been investigated by synergy of Fourier transform infrared (FTIR) spectroscopy and small angle neutron scattering (SANS) experiments. By focusing on the influence of temperature as external stimulus and block length asymmetry, differences in morphologies and molecular hydration characteristics of two PNIPAM-b-POEGA diblock copolymers were resolved. With increasing temperature, the macromolecular structures undergo block-length dependent transformations from hierarchical assemblies to more well-defined spherical morphologies as evidenced by SANS. Differences in the strength and/or amount of hydrogen bonding and hydrophobic interactions lead to distinct morphological transformations expressed by variations in cluster compactness and hydration. In these assemblies of PNIPAM-b-POEGA with the short PNIPAM block, the methyl side group hydration, as evidenced by FTIR, sensitively depends on the temperature increase at temperatures even beyond the nominal volume phase transition temperature. For both blocks, the evolution of the amide I band reflects that solvent-polymer interactions are still favorable even at the highest temperatures. The understanding of these assemblies provides ground for optimization of these scaffolds for drug encapsulation protocols.

Primary authors: VAGIAS, Apostolos (FRM2 / TUM); MÜLLER-BUSCHBAUM , Peter (1 Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany 2 Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany); BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); Dr PISPAS, Stergios (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece); Mrs GIAOUZI, Despoina (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens, Greece); KREUZER, Lucas (MLZ (FRM II, TUM)); Dr PAPAGIANNOPOULOS, Aris (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens, Greece)

Presenter: VAGIAS, Apostolos (FRM2 / TUM)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **110** Type: **Poster**

Superstructure in inverse perovskite nitrides

Wednesday, December 8, 2021 10:30 AM (1h 30m)

We are investigating the crystal structure and properties of inverse perovskite nitrides with elpasolite-type superstructures. This superstructure is due to a full or partial ordering of nitrogen atoms and defects on the perovskite B site. Since nitrogen scatters neutrons much more strongly than X-rays, neutron diffraction measurements of seven compounds with this superstructure were performed. Beforehand, we had illuminated their crystal structures using X-ray powder diffractometry, but were unable to determine the exact nature and extent of the superstructure.
After neutron diffraction measurements, the superstructures could be modeled much more reliably by simultaneous refinement of X-ray and neutron data, utilizing the advantages of both methods. For $(Sr_3N_{0.5})Ge$, $(Ba_3N_{0.5})Ge$, $(Ba_3N_{0.5})Sn$ and $(Ba_3N_{0.5})Pb$, a full ordering of nitrogen and vacancies was confirmed. In contrast, analogous calcium compounds have a higher nitrogen content and show only partial ordering. One of the elpasolite B sites is fully occupied by nitrogen in every case. Most of the crystal structures feature octahedral tilting, which leads to an inverse $Na_3[AlF_6]$-type structure for $(Ca_3N_{0.69})Ge$, $(Sr_3N_{0.5})Ge$ and $(Ba_3N_{0.5})Ge$. $(Ba_3N_{0.5})Sn$ and $(Ba_3N_{0.5})Pb$ crystallize in space group $R\overline{3}$ with less pronounced tilting, while the inverse $K_2(NaAlF_6)$-type structure of $(Ca_3N_{0.65})Sn$ and $(Ca_3N_{0.56})Pb$ has no octahedral tilting.

Primary author: LINK, Lukas

Co-authors: NIEWA, Rainer (Universität Stuttgart); BARAN, Volodymyr (DESY, FS-PETRA-D, P02.1); Dr HANSEN, Thomas (Institut Laue-Langevin Grenoble)

Presenter: LINK, Lukas

Session Classification: Poster Session II

Track Classification: Structure Research

Contribution ID: **111** Type: **Talk**

Structural and thermophysical properties of undercooled glass forming CuTi melts

Tuesday, December 7, 2021 9:55 AM (25 minutes)

CuTi-based glass forming alloys feature a large undercooled liquid region and a high glass-forming ability, which makes them interesting materials particularly for biomedical and lightweight applications. However, for the development of alloy compositions with optimized glass-forming abilities, the relevant mechanisms on the atomic scale are still to be explored. For a fundamental understanding of the glass formation processes, regarding the atomic structures and short-range orders in the undercooled melt, binary CuTi serves as a less complex reference system. We studied composition-dependent packing fraction and short-range order in the binary CuTi liquids in the range of 33 to 76 at% Cu by neutron and x-ray diffraction. Due to the high chemical reactivity of Ti-based melts, the CuTi samples have been containerlessly processed using electrostatic levitation. This technique enables access to the metastable regime of an undercooled melt. In addition, the absence of any container or crucible results in an excellent signal-to-noise ratio in scattering experiments. To take full advantage of the different scattering contrasts of the CuTi system, data from neutron scattering and diffraction with synchrotron radiation are combined, which gives information on topological and chemical short-range orders. The atomic structure is brought into correlation with the thermophysical properties such as the melt viscosity, which reflect the dynamic behavior of the system.

Primary authors: Dr KREUZER, Lucas (1MLZ (FRM II, TUM), 2Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR)); Dr YANG, Fan (Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR)); Dr EVENSON, Zach (2Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR)); Dr HOLLAND-MORITZ, Dirk (Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR)); Dr BERNASCONI, Andrea (European Synchrotron Radiation Facility (ESRF)); Dr HANSEN, Thomas (Institut Laue-Langevin (ILL)); Prof. MEYER, Andreas (Institut Laue-Langevin (ILL), 2Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR)); Prof. PETRY, Winfried (FRM II - TUM)

Presenter: Dr KREUZER, Lucas (1MLZ (FRM II, TUM), 2Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR))

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **112** Type: **Poster**

Investigation of magnetic domains in [Pt/Co/Ta]10 multilayers using magnetic force microscopy

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Multilayers composed of heavy metals and ferromagnets with strong perpendicular anisotropy are potential candidates for magnetic memory applications [1,2]. Magnetic skyrmions in particular may enable ultra-dense storage devices due to their extremely low spin currents [2]. Pt/Co-based multilayers generally exhibit worm domains, which can nucleate into domains of skyrmions through breaking/nucleation processes [3,4]. Recent studies have demonstrated the nucleation of skyrmions by varying external magnetic field, temperature and current in Pt/Co/Ta multilayers prepared by sputtering [4,5].
In this work, [Pt/Co/Ta]10 multilayers with cobalt layer thickness between 5 Å to 21 Å were grown by molecular beam epitaxy. We assessed the dependence of the magnetic domain structure on the cobalt thickness of [Pt/Co/Ta]10 multilayers by means of magnetic force microscopy (MFM). The magnetic domains were manipulated by applying different magnetic fields and measuring either in field or in remanence. The results of the systematic investigation are presented and discussed in detail.

References:
1 A. Fert and V. Sampai, Nat. Nanotechnol. 8 (2013) 152–156
[2] C. Wang et al., J. Phys. D: Appl. Phys. 46 (2013) 285001
[3] M. Ma et al., J. Appl. Phys. 127 (2020) 223901
[4] J. Brandao et al., Appl. Nano Mater. 2 (2019) 7532–7539
[5] S. Zhang et al., Appl. Phys. Lett. 112 (2018) 132405

Primary author: MONTANEZ HUAMAN, Liz Margarita

Co-author: PÜTTER, Sabine (Jülich Centre for Neutron Science JCNS, Outstation at MLZ, Forschungszentrum Jülich GmbH)

Presenter: MONTANEZ HUAMAN, Liz Margarita

Session Classification: Poster Session

Track Classification: Quantum Phenomena

Contribution ID: **113** Type: **Talk**

166-Ho Quiremspheres for treating unresectable liver tumors

Tuesday, December 7, 2021 9:55 AM (25 minutes)

Quirem Medical BV, a Terumo company, is the manufacturer and supplier of holmium-166 (Ho-166) microspheres. These radioactive microspheres are used for Selective Internal Radiation Therapy (SIRT) which is one of the treatment options for liver tumors. Via placement of a microcatheter in the liver artery of the patient, the microspheres are injected into the blood stream. These microspheres lodge in the small vessels surrounding the tumor and emit β-radiation to irradiate the tissue. Beside emitting β-radiation, the holmium microspheres have two other unique properties: Ho-166 emits γ-radiation and the material is paramagnetic, allowing to perform SPECT and MR imaging respectively. Based on these imaging methods, the distribution of the Ho-166 microspheres throughout the liver can be accurately assessed. The activation of Ho-166 inside the microspheres is reached by the neutron irradiation in the nuclear research reactors. The microspheres are packed in specific developed irradiation capsules and irradiated up to the requested activity level. The FRM II reactor has demonstrated to be a valuable and constructive partner in the development of this irradiation process to activate the Ho-166 microspheres. The rabbit post pneumatic irradiation facility RPA has been successfully applied for these purposes. Since 2016, FRM II is successfully activating Ho-166 microspheres for patient treatments throughout Europe. We plan to continue our collaboration also after reactor restart 2022.

Primary author: Mr VAN WOLFWINKEL, Gerhard (Quirem Medical B.V.)

Co-authors: Dr HUTANU, Vladimir (ZWE FRM II, TUM); Mr JESCHKE, Florian (ZWE FRM II, TUM)

Presenter: Mr VAN WOLFWINKEL, Gerhard (Quirem Medical B.V.)

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **114** Type: **Poster**

STRUCTURE AND MAGNETISM IN MULTILAYER Fe/MgO/Cr/MgO/Fe NANOSYSTEMS

Tuesday, December 7, 2021 10:30 AM (1h 30m)

Layered Fe/MgO/Cr/MgO/Fe nanostructures are an artificial ferromagnetic material in which the exchange interaction of magnetic moments of Fe layers through intermediate dielectric and metal layers can lead to magnetic configurations that are not realized in the well-studied Fe/MgO/Fe and Fe/Cr/Fe systems. The correlation between the structural and magnetic properties of layered Fe(10 nm)/MgO(1.5 nm)/Cr(t)/MgO(1.5 nm)/Fe(7 nm) (t = 0.9 and 1.8 nm) nanoheterostructures was studied. X-ray diffractometry and high-resolution reflectometry data confirmed the formation of an epitaxial crystal structure and revealed its well-defined layered nature with sharp interlayer boundaries. Vibration magnetometry did not reveal significant differences in the hysteresis loops of a characteristic stepped shape. Reflectometry of polarized neutrons made it possible to establish that the processes of magnetization reversal in these samples occured in different ways at the level of individual Fe layers. In the sample with a 0.9 nm thick Cr interlayer, the Fe layers were exchange-coupled through the MgO/Cr/MgO interlayer, and their rotation was correlated with the application of a magnetic field. In the sample with a 1.8 nm thick Cr interlayer, the Fe layers were not exchange-coupled and magnetized independently of each other. It was found that the magnetization reversal of the Fe/MgO/Cr/MgO/Fe systems was characterized by an intermediate state, which could be controlled using a small external field of several tens of oersted and a change in the orientation of the sample, as well as by varying the thickness of the MgO layer.

Primary author: Ms YAKUNINA, Elena (Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences)

Co-authors: KRAVTSOV, Evgeny; ANTROPOV, Nikolay; Mr PROGLYADO, Vyacheslav (Institute of Metal Physics); KHAYDUKOV, Yury

Presenter: Ms YAKUNINA, Elena (Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences)

Session Classification: Poster Session

Track Classification: Quantum Phenomena

Contribution ID: **115** Type: **Talk**

New Perspectives for Neutron Imaging through Advanced Event-Mode Data Acquisition

Tuesday, December 7, 2021 2:05 PM (25 minutes)

Recently developed event-driven detectors are capable of registering spots of light induced by neutron interactions in scintillator materials. Reconstructing the Center-of-Mass of the individual interactions, it is possible to significantly enhance spatial and temporal resolution of recorded radiographs. Utilizing this principle, we present a detector capable of Time-of-Flight imaging with an adjustable field-of-view, ad-hoc binning and re-binning of data based on the requirements of the experiment including the possibility of particle discrimination via the analysis of the event shape in space and time. It is considered that this novel concept might replace regular cameras in neutron imaging detectors as it provides superior detection capabilities compared to conventional frame-based camera systems.

Primary author: Dr LOSKO, Adrian (Heinz Maier-Leibnitz Zentrum)

Co-authors: Dr HAN, Yiyong (Heinz Maier-Leibnitz Zentrum); Dr SCHILLINGER, Burkhard (Heinz Maier-Leibnitz Zentrum); Dr TARTAGLIONE, Aureliano (Heinz Maier-Leibnitz Zentrum); Dr MORGANO, Manuel (Paul Scherrer Institut); Dr STROBL, Markus (Paul Scherrer Institut); Dr LONG, Jingming (Amsterdam Scientific Instruments); Dr TREMSIN, Anton (University of California); Dr SCHULZ, Michael (Heinz Maier-Leibnitz Zentrum)

Presenter: Dr LOSKO, Adrian (Heinz Maier-Leibnitz Zentrum)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **116** Type: **Talk**

Spin dynamics in Multiferroic Ba2CoGe2O7

Tuesday, December 7, 2021 5:05 PM (25 minutes)

Multiferroic $Ba_2CoGe_2O_7$ belongs to the square lattice Heisenberg antiferromagnets (SLHAF), which exhibit rich quantum phase diagrams of exchange interactions, Dzyaloshinskii-Moriya interactions with the external magnetic or electric fields, but the correlation between single-ion anisotropy and the magnetic field has remain hitherto unexplored through experimental findings in multiferroic quantum materials. we present very compelling and direct evidence of the anisotropic three-dimensional (3D) magnetic excitations in $Ba_2CoGe_2O_7$ for the first time, using Inelastic neutron scattering under magnetic fields upto 12 T. Additionally, we show the a pair of electromagnon modes (so far one mode has reported) are indeed dispersive in 3D and also responsive to the applied magnetic field as well. Most strikingly, here we present that the underlying strong single-ion anisotropy gets minimized or, tuned under the action of external magnetic field [R. Dutta et al., Phys. Rev. B 104, L020403]. In our believe, such tuning of single-ion anisotropy under magnetic field will bring a novel insight into the physics of general quantum phenomena towards also the multiferroic device applications point of view as the SIA could be tuned by an external electric field like in single-ion magnets or single-molecular magnets.

Primary author: Dr DUTTA, Rajesh (Institut für Kristallographie, RWTH Aachen University)

Presenter: Dr DUTTA, Rajesh (Institut für Kristallographie, RWTH Aachen University)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **117** Type: **Poster**

Design, Fabrication and Nano-Scale Characterization of Novel SEI Layers

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Rechargeable lithium metal batteries have been recognized one of the most promising energy storage devices due to their superior energy density. However, serious safety concern and poor cyclability are featured originating from uncontrolled lithium dendrite growth and unstable solid electrolyte interface (SEI) layer. One strategy to suppress dendrite growth is surface modification with Amphiphilic block copolymers, such as PDMS-b-PAA, which bear some clear advantages including absorbing mechanical stress, conducting lithium ion, controling the lithium dendrite growth process. With scattering techniques using neutrons and in situ scattering studies, the structures of the surface modified lithium metal anodes and structure formation processes can be studied. Moreover, by applying GISANS, the horizontal structures and vertical structures of the polymer films on the lithium metal surfaces can be investigated reflectivity.

Primary author: XU, Zhuijun (Technische Universität München)

Co-authors: Prof. MÜLLER-BUSCHBAUM, Peter (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien); Prof. CHENG, Yajun (Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences); Prof. XIA, Yonggao (Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences,)

Presenter: XU, Zhuijun (Technische Universität München)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **118** Type: **Plenary talk**

Responding a challenge: remote access and digital twins at MLZ

Wednesday, December 8, 2021 4:05 PM (20 minutes)

The COVID-19 crisis has created new challenges worldwide. On the plus side, it has been a catalyst for digitalization, also at the MLZ. Besides providing remote access to our instrument control- and data analysis systems, online training has become increasingly important. In January 2021, the first lab course with students were carried out online, using so-called Digital Twins. A Digital Twin is a virtual representation of an instrument, in particular a simulation of the neutron scattering at the sample with varying input parameters. This talk gives an overview of the current state of digital twinning at MLZ, including a live demonstration and future prospects regarding using Digital Twins beyond educational purposes.

Primary author: FELDER, Christian

Presenter: FELDER, Christian

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **119** Type: **Talk**

Orbital Angular Momentum Generation in the Neutron-Nucleus Weak Interaction

Tuesday, December 7, 2021 2:05 PM (25 minutes)

During the 1970s parity non-conserving spin rotations where first observed in the neutron nucleus weak interaction 1. In these experiments transversally polarized neutrons were passed through certain nuclear targets, upon which the neutron spin was rotated around the flight direction. Due to the conservation of total angular momentum this spin rotation has to be compensated in some manner. In contrast to the magnetic interaction, where total angular momentum is conserved by transferring some angular momentum to the magnet, the formalism of the neutron nucleus weak interaction [2] seems to indicate total angular momentum is conserved by imprinting orbital angular momentum (OAM) on the neutron. In the proposed talk arguments for neutron orbital OAM generation are derived from the formalism of the neutron nucleus weak interaction. Furthermore, we present an experimental scheme by which this OAM can be observed in a polarized neutron diffractometer. Finally, preliminary experimental evidence is shown in which a spin-OAM coupled neutron state [3] is passed through a Lanthanum target. The data appears to confirm conservation of the total neutron angular momentum within experimental accuracy.

1: M. Forte et al., PRL, 45 2088-2092, 1980.
[2]: F.C. Michel. Phys Rev., 133 329-349, 1964.
[3]: J. Nsofini et al., Phys. Rev. A 94, 013605 2016.

Primary author: GEERITS, Niels (TU Wien, Atominstitut)

Co-authors: STEFFEN, Kyle (Indiana University); Prof. SNOW, William Michael (Indiana University); Dr SPONAR, Stephan (Atominstitut TU Wien)

Presenter: GEERITS, Niels (TU Wien, Atominstitut)

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **120** Type: **Poster**

Structure and dynamics of supramolecular poly(ethylene) oxide polymer blends

Wednesday, December 8, 2021 10:30 AM (1h 30m)

In this work, we present a combined analysis of small angle neutron scattering (SANS), linear rheology and neutron spin eco (NSE) spectroscopy experiments on the supramolecular association and chain structure of supramolecular polymer blends. These consist of well-defined hydrogenated (H) polymers with a polyethylene oxide (PEO) backbone carrying the directed homocomplementary hydrogen-bonding functional end-group, ureidopyrimidinone (upy), immersed in their own deuterated (D) covalent short linear non-functionalized PEO chains in the melt as solvent. The molar mass (MW) of the functionalized (H) PEO is 2000 gmol-1, and of the non-functionalized (D) PEO chains 500 gmol-1. Their self-assembly and phase behavior in the melt state is investigated as a function of temperature and supramolecular polymer mass fraction in the ideal blend. It is found that on contrary to the bulk structure in the melt 1, the supramolecular polymer in the blend is well described by the Gaussian model. In particular, the conformation of the supramolecular polymer in the blend changed from linear to ring -like with increasing supramolecular polymer mass fraction. These findings are also confirmed by the NSE analysis with the modified Rouse model for ring polymers from which the expected diffusion and segmental friction is obtained [2,3].

A.B. acknowledges DFG for a research grant (BR5303) and Prof. D. Richter for discussions

1 A. Brás, A. Arizaga, U. Agirre, M. Dorau, J. Houston, A. Radulescu, M. Kruteva, W. Pyckhout-Hintzen, A. M. Schmidt, Polymers 2021, 13, 2235.
[2] A. R. Brás, R. Pasquino T. Koukoulas G. Tsolou, O. Holderer, A. Radulescu, J. Allgaier, V. G. Mavrantzas W. Pyckhout-Hintzen, A. Wischnewski, D. Vlassopoulos, D. Richter Soft Matter, 2011, 7, 11169.
[3] K. Niedzwiedz, A. Wischnewski, W. Pyckhout-Hintzen, J. Allgaier, D. Richter , A Faraone, Macromolecules, 2008, 13, 4866.

Primary author: BRÁS WÜRSCHIG, Ana (Institute of Physical Chemistry, University of Cologne)

Co-authors: Dr ARIZAGA, Ana (Institute of Physical Chemistry, University of Cologne); Mrs BACH, Patricia (Institute of Physical Chemistry, University of Cologne); Dr RADULESCU, Aurel (Jülich Centre for Neutron Science (JCNS-1) at Heinz Maier Leibnitz-Zentrum (MLZ), Forschungszentrum Jülich GmbH); Dr HOFFMANN, Ingo (Institute Laue Langevin (ILL)); Dr KRUTYEVA, Margarita (Jülich Centre for Neutron Science (JCNS-1), Forschungszentrum Jülich GmbH); Dr MONKENBUSCH, Michael (Jülich Centre for Neutron Science (JCNS-1), Forschungszentrum Jülich GmbH); Dr PYCKHOUT-HINTZEN, Wim (Jülich Centre for Neutron Science (JCNS-1), Forschungszentrum Jülich GmbH); Prof. SCHMIDT, Annette M. (Institute of Physical Chemistry, University of Cologne)

Presenter: BRÁS WÜRSCHIG, Ana (Institute of Physical Chemistry, University of Cologne)

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **121** Type: **Talk**

On the analyses of grazing incidence small angle neutron scattering patterns arising from regular nanostructured arrays

Tuesday, December 7, 2021 4:15 PM (25 minutes)

We report a new, simplified approach for analysis of grazing incidence scattering measurements used to investigate supported lipid bilayers on hexagonal arrays of nanowires. The method exploits measurements of different physical structures or different scattering contrasts in studies of a fixed array of nanowires. The ratio of the intensity at peaks can be calculated for models simply as a ratio of form factors or scattering functions for the different conditions. The ratios of experimentally measured peak intensities are compared with models to provide structural information. Direct consideration of the ratios of observed intensities avoids many complications of quantitative calculation of grazing incidence scattering that are related to resolution, depth of penetration, refraction, and background scattering. The present work enables the determination of the thickness and density of a mixed lipid layer formed by vesicle fusion on the curved surface of nanowires which can be directly compared with that on the flat substrate between the nanowires. Suggestions for further developments of this methodology are provided.

Primary authors: Dr MOTHANDER, Karolina (Lund University); Prof. PRINZ, Christelle (Lund University); Prof. NYLANDER, Tommy (Lund University); Prof. RENNIE, Adrian (Uppsala University)

Presenter: Prof. NYLANDER, Tommy (Lund University)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **122** Type: **Poster**

Neutron diffraction studies of compounds based on MnGe under high pressure at low temperatures in high magnetic fields

Tuesday, December 7, 2021 10:30 AM (1h 30m)

The creation of extreme conditions on the sample by means of high external pressure together with changes in the magnetic field and temperature allows to obtain the comprehensive amount of experimental data for a detailed description of the internal properties of materials.
We investigated the $Mn_{1-x}Fe_xGe$ compounds, which crystallize into a noncentrosymmetric cubic structure of the B20 type, with Small-angle neutron scattering (SANS) under applied pressure and high magnetic field. In order to perform the corresponding study, the nonmagnetic high-pressure cell was developed that fits the standard sample position and allows to increase the pressure up to 12 kbar with possibility of further improvement up to 25 kbar. The ambient pressure experiment was performed at SANS-1 at FRM-II, while the high-pressure experiment was fulfilled at SANS diffractometer PA20, which was located at LLB, Saclay, France.
On the basis of the obtained experimental data, it becomes possible to estimate the real influence of a change of the cell constant, without taking into account the change in the electron concentration, on the evolution of the field-temperature phase diagram for compounder under investigation.

Primary authors: SKANCHENKO, Daria (NRC «Kurchatov Institute» - PNPI); Dr ALTYNBAEV, Evgeny (NRC «Kurchatov Institute» - PNPI); Dr SADYKOV, Ravil (Institute of Nuclear Research, Russian Academy of Sciences); Dr MARTIN, Nicolas (CNRS, Laboratoire Léon Brillouin); TSVYASCHENKO, Anatoly (Vereshchagin Institute for High Pressure Physics, Russian Academy of Sciences); Prof. GRIGORIEV, Sergey (NRC «Kurchatov Institute» - PNPI)

Presenter: SKANCHENKO, Daria (NRC «Kurchatov Institute» - PNPI)

Session Classification: Poster Session

Track Classification: Quantum Phenomena

Contribution ID: **123** Type: **Poster**

Elemental characterization by PGAA to support decommissioning activities

Wednesday, December 8, 2021 10:30 AM (1h 30m)

The implementation of decommissioning tasks requires accurate radiological characterization to be accomplished. Often, computational codes are used to complement experimental radiological characterization campaigns. These activation codes need accurate knowledge of elemental composition of non-irradiated materials. Besides determination of most nuclides by the well-established Inductively Coupled Plasma – Mass Spectrometry (ICP-MS), Prompt Gamma Activation Analysis (PGAA) may be helpful in measuring light elements such as B, N, and Cl, that are known to be important precursors for medium (3H) and long-lived (14C and 36Cl) neutron activation radionuclides. In fact, the assessment of N and Cl by ICP-MS is nearly impossible, whenever HNO3 and HCl are employed to dissolve the sample.
The aim of this work is to complete the elemental characterization of nuclear grade graphite used as moderator and reflector in L-54M nuclear research reactor operated by Politecnico di Milano and now in deferred dismantling decommissioning. The bulk concentrations measured by PGAA resulted to be in agreement with ICP-MS and literature data, when available. Moreover, for the first time, depth distribution concentration profiles of N and Cl have been demonstrated. All data obtained by this innovative approach will be fed into the formerly developed activation code to accurately calculate radionuclides distribution in real samples and support their characterization before decommissioning.

Primary authors: MOSSINI, Eros (Politecnico di Milano); Mr REVAY, Zsolt (MLZ); Mr CAMERINI, Andrea (Politecnico di Milano); Ms MACERATA, Elena (Politecnico di Milano); Mr MARIANI, Mario (Politecnico di Milano)

Presenter: MOSSINI, Eros (Politecnico di Milano)

Session Classification: Poster Session II

Track Classification: Neutron Methods

Contribution ID: **124** Type: **Talk**

On the reliability of phase-specific residual stress analyses on textured, multiphase materials using diffraction methods - Example: Duplex stainless steels

Tuesday, December 7, 2021 4:15 PM (25 minutes)

Process-induced residual stresses (RS), which are induced as a result of plastic deformation, can lead to plastic anisotropy effects caused by intergranular strains. The strict application of diffraction elastic constants (DEC) to calculate phase-specific RS, as tabulated for many material phases in literature, can lead to arguably erroneous RS calculations. These plastic anisotropy effects can be numerically calculated taking into account phase-specific textures, e.g. by means of EPSC modelling (elasto-plastic self-consistent modelling).
EPSC simulations were carried out for the two duplex stainless steels X2CrNiMoN22-5-3 and X3CrNiMoN27-5-2, which differ in their ratio of ferrite to austenite and in the phase-specific textures. A distinction is made between the cases with and without texture and the corresponding deviations were determined and discussed. The numerically determined results are compared with results from in situ neutron diffraction experiments determined for uniaxially loaded tensile specimens at different neutron diffraction experiments (MLZ, ILL, ISIS). Finally, a practical application of the findings to the neutronographic determination of the RS depth distribution is carried out on the deep-rolled duplex steel X2CrNiMoN22-5-3. In the discussion of the results, a comparison is made with results from complementary RS analyses using the incremental hole drilling method and from X-ray RS analysis according to the well-known sin²968;-method.

Primary authors: Mr PULVERMACHER, Samuel (Karlsruher Institut für Technologie, IAM-WK); Dr GIBMEIER, Jens (Karlsruher Institut für Technologie, IAM-WK); Dr HOFMANN, Michael (Heinz Maier-Leibnitz Zentrum (MLZ), TU München); Dr REBELO KORNMEIER, Joana (Heinz Maier-Leibnitz Zentrum (MLZ), TU München); Dr SAROUN, Jan (Nuclear Physics Institute of the CAS)

Presenter: Dr GIBMEIER, Jens (Karlsruher Institut für Technologie, IAM-WK)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **125** Type: **Talk**

Status of the neutron decay facility PERC

Tuesday, December 7, 2021 4:15 PM (25 minutes)

For the PERC Collaboration.

The Proton Electron Radiation Channel (PERC) instrument aims to measure several observables in neutron decay with unprecedented precision. It will serve to determine parameters within the Standard Model of particle physics and to search for novel scalar and tensor interaction beyond it. Together with precision measurements of the neutron lifetime, results will be used to determine the first element of the quark-mixing CKM matrix V_{ud} free from nuclear effects with competitive precision.

With the delivery of the main component, a twelve meter long superconducting magnet system, to the new beam site Mephisto in the guide hall east, a major milestone of the project has been achieved. We present the status of the project and the road to first science.

Primary author: MÄRKISCH, Bastian (Physik-Department, TUM)

Presenter: MÄRKISCH, Bastian (Physik-Department, TUM)

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **126** Type: **Talk**

Gas adsorption studied by in situ powder diffraction: from structural evolution to thermodynamics

Tuesday, December 7, 2021 9:05 AM (25 minutes)

In this presentation I will show examples of using in situ powder diffraction to simultaneously access the structure and adsorption properties of a small pore crystalline solid. (Quasi)-equilibrium isotherms and isobars can be built directly from sequential Rietveld refinements, both on adsorption and desorption, thus addressing the hysteresis and kinetics of gas adsorption/desorption. Detailed picture of guest reorganization with an increasing uptake can be obtained.
We investigated gas sorption in the porous γ-Mg(BH4)2 using neutron powder diffraction to accurately localize the guests and synchrotron X-ray powder diffraction to collect data along the adsorption isobars. The latter allows to study structural changes with pressure and temperature variation, giving insight into guest-host and guest-guest interactions, as well as to extract relevant thermodynamic parameters. I will discuss the intermolecular interactions, size effects and the role of hydridic hydrogen in physisorption. In this small-pore system, the effect of the probe size on the loading capacity and the location of the guest molecules is remarkable. While typically each pore can be occupied by one or two larger guests, the amount of hydrogen can go up to 5 molecules per pore, yielding the total capacity of 2.33 H2 molecules per Mg atom.

Primary author: FILINCHUK, Yaroslav (Université catholique de Louvain)

Presenter: FILINCHUK, Yaroslav (Université catholique de Louvain)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **127** Type: **Poster**

Silicon detector for neutron beta decay measurements with PERC

Wednesday, December 8, 2021 10:30 AM (1h 30m)

The PERC facility is currently under construction at the MEPHISTO beamline of the FRM II. It will serve as an intense and clean source of electrons and protons from neutron beta decay for precision studies. It aims to improve the measurements of the properties of weak interaction by one order of magnitude and to search for new physics via new effective couplings.
PERC's central component is a 12 m long superconducting magnet system that has recently been delivered. It hosts an 8 m long decay region in a uniform field. An additional high-field region selects the phase space of electrons and protons, which can reach the downstream detector and systematic uncertainties.
The downstream main detector and the two upstream backscattering detectors, will initially be scintillation detectors with (silicon) photomultiplier readout. In a later upgrade, the downstream detector will be replaced by a pixelated silicon detector. We present the current design status of the silicon detector prototype.

Primary author: LEBERT, Manuel (Technical University Munich)

Co-authors: LAMPARTH, Max (TUM); KLENKE, Jens (FRM II); BERNERT, Karina (TUM); MÄRKISCH, Bastian (Physik-Department, TUM)

Presenter: LEBERT, Manuel (Technical University Munich)

Session Classification: Poster Session II

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **128** Type: **Poster**

Dynamic structure evolution of extensively de-lithiated high voltage spinel Li1+xNi0.5Mn1.5O4 x<1.5

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Nickel manganese spinel LiNi0.5Mn1.5O4 is considered one of the most promising cathode materials for lithium-ion batteries. On the one hand, this is because of its high energy density due to its high voltage plateau at 4.7 V, and the high rate capability due to its three dimensional diffusion network in the cubic crystal system. On the other hand, this material is interesting because additional lithium can be incorporated into the crystal system by exploiting the redox chemistry of manganese, rather than using only the nickel. This feature can be used to compensate for losses in the initial cycles or to increase the overall capacity and energy density even further.
However, the extensive lithiation to Li2.5Ni0.5Mn1.5O4 in the complete voltage range from 4.9 V to 1.5 V leads to an aging of the material and capacity fading. In order to tackle this problem it is necessary to provide answers to two questions: Are there intermediate phases that can be identified and where is lithium intercalated to when all octahedral site in the spinel are occupied, at x>2 in LixNi0.5Mn1.5O4.
By applying potentiometric entropymetry and operando XRD, we were able to reveal a simultaneous formation of Li2Ni0.5Mn1.5O4 and Li2.5Ni0.5Mn1.5O4, both with tetragonal I41amd space group, but with large c and small a and b lattice parameters. Via neutron diffraction we where able to locate the additional lithium on octahedral 8a and tetrahedral 4a positions of the distorted tetragonal phase I41amd. Furthermore, the neutron diffraction revealed a partial site exchange of lithium and nickel ions. This observation could be identified as one aging mechanism for the material by perfoming post mortem XRD measurements on aged LiNi0.5Mn1.5O4 based electrodes.

Primary author: JOBST, Nicola (ZSW)

Co-authors: PAUL, Neelima (Technical University of Munich, Heinz Maier-Leibnitz Zentrum (MLZ)); BERAN, Premysl (Nuclear Physics Institute CAS); GILLES, Ralph (MLZ TUM)

Presenter: JOBST, Nicola (ZSW)

Session Classification: Poster Session II

Track Classification: Material Science

Contribution ID: **129** Type: **Talk**

Garnet to hydrogarnet: effect of post synthesis treatment on cation substituted LLZO solid electrolyte and its effect on Li ion conductivity

Tuesday, December 7, 2021 1:40 PM (25 minutes)

We investigated why commercial Li7La3Zr2O12 (LLZO) with Nb- and Ta substitution shows very low mobility on a local scale, as observed with temperature-dependent NMR techniques, compared to Al and W substituted samples, although impedance spectroscopy on sintered pellets suggests something else: conductivity values do not show a strong dependence on the type of substituting cation. We observed that mechanical treatment of these materials causes a symmetry reduction from garnet to hydrogarnet structure. To understand the impact of this lower symmetric structure in detail and its effect on the Li ion conductivity, neutron powder diffraction and 6Li NMR were utilized. Despite the finding that, in some materials, disorder can be beneficial with respect to ionic conductivity, pulsed-field gradient NMR measurements of the long-range transport indicate a higher Li+ diffusion barrier in the lower symmetric hydrogarnet structure. The symmetry reduction can be reversed back to the higher symmetric garnet structure by annealing at 1100 ℃. This unintended phase transition and thus a reduction in conductivity is crucial for the processing of LLZO materials in the fabrication of all-solid state batteries.

Primary authors: FRITSCH, Charlotte; Dr ZINKEVICH, Tatiana; Dr INDRIS, Sylvio; Dr ETTER, Martin; BARAN, Volodymyr (DESY, FS-PETRA-D, P02.1); Dr BERGFELDT, Thomas; EHRENBERG, Helmut (KIT); KNAPP, Michael (KIT, IAM-ESS); Dr HANSEN, Anna-Lena

Presenter: FRITSCH, Charlotte

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **130** Type: **Plenary talk**

DAPHNE4NFDI: DAta from PHoton and Neutron Experiments for NFDI

Wednesday, December 8, 2021 3:45 PM (20 minutes)

The photon and neutron science community encompasses users from a broad range of scientific disciplines. With the advent of high speed detectors and increasingly complex instrumentation, the user community faces a common need for high-level, rapid data analysis and the challenge of implementing research data management for increasingly large and complex datasets. The aim of DAPHNE4NFDI is to create a comprehensive infrastructure to process research data from large scale photon and neutron infrastructures according to the FAIR principles (Findable, Accessible, Interoperable, Repeatable).

DAPHNE4NFDI brings together users representing key scientific application domains with the large-scale research facilities in photon and neutron science in order to advance the state of data management in the community. Key tasks to be addressed within DAPHNE4NFDI are
- Improve metadata capture through consistent workflows supported by user-driven online logbooks that are linked to the data collection;
- Establishment of community repositories processed data, new reference databases and analysis code for published results, linked, where possible, to raw data sources, to sustainably improve access to research data; and
- Develop, curate and deploy user-developed analysis software including the interface for machine learning tools on facility computing infrastructure through common data analysis portals.

Financed through the Deutsche Forschungsgemeinschaft National Research Data Infrastructure programme, DAPHNE4NFDI aims to have impact across the wider European and international photon and neutron community.

Primary authors: BARTY, Anton (DESY); BUSCH, Sebastian (MLZ - Hereon); GRUNWALDT, Jan-Dierk (Karlsruhe Institut für Technologie (KIT)); GUTT, Christian (Universität Siegen); MURPHY, Bridget (CAU Kiel); SCHNEIDEWIND, Astrid (MLZ - JCNS); SCHREIBER, Frank (Universität Tübingen); UNRUH, Tobias (FAU Erlangen Nürnberg); LOHSTROH, Wiebke (MLZ - Technische Universität München)

Presenter: LOHSTROH, Wiebke (MLZ - Technische Universität München)

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **131** Type: **Talk**

Compositional Studies of Metals with Complex Order by means of the Optical Floating-Zone Technique

Tuesday, December 7, 2021 4:40 PM (25 minutes)

The availability of large high-quality single crystals is an important rerequisite for many studies in solid-state research. The optical floating-zone technique is an elegant method to grow such crystals, offering potential to prepare samples that may be hardly accessible with other techniques. As elaborated in this presentation, examples include single crystals with intentional compositional gradients, deliberate off-stoichiometry, or complex metallurgy. For the cubic chiral magnets Mn1−xFexSi and Fe1−xCoxSi, single crystals are prepared in which the composition is varied during growth from x = 0 to 0.15 and from x = 0.1 to 0.3, respectively. Such samples allow us to efficiently study the evolution of the magnetic properties as a function of composition, as demonstrated by means of neutron scattering. For the archetypical chiral magnet MnSi and the itinerant antiferromagnet CrB2, single crystals with varying initial manganese (0.99–1.04) and boron (1.95–2.1) content are grown. Measurements of the low-temperature properties address the correlation between magnetic transition temperature and sample quality. Furthermore, single crystals of the diborides ErB2, MnB2, and VB2 are prepared. In addition to high vapor pressures, these materials suffer from peritectic formation, potential decomposition, and high melting temperature, respectively.

Primary authors: BAUER, Andreas (Technische Universität München); Dr BENKA, Georg; Mr ENGELDARDT, Alexander; Dr NEUBAUER, Andreas; Dr REGNAT, Alexander; Mr RESCH, Christoph; Dr WURMEHL, Sabine; Mr BLUM, Christian G. F.; Dr ADAMS, Tim; Dr CHACON, Alfonso; Dr JUNGWIRTH, Rainer; Dr GEORGII, Robert; Dr SENYSHYN, Anatoliy; Dr PEDERSEN, Björn; Dr MEVEN, Martin; Prof. PFLEIDERER, Christian

Presenter: BAUER, Andreas (Technische Universität München)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **132** Type: **Poster**

Self-assembly of polymer coated iron oxide nanoparticles in magnetic field

Wednesday, December 8, 2021 10:30 AM (1h 30m)

Functional nanocomposites are an important class of smart and adaptive materials. They offer a broad application range from sensors through stretchable electronics to energy conversion and human health. Especially, responsive materials which are able to perform self-assembly in different environments (e.g. magnetic field) are in the center of interest. Further developments in this area would significantly benefit from deeper insights into the self-assembly of the nanoparticles depending on the temperature, external field strength, initial distance between particles etc.

Iron oxide nanoparticles grafted with polymer play the significant role in creating magnetically tunable photonic crystal systems. Self-assembly of these nanocomposites can be controlled by varying the core-polymer shell size and the strength of external field. In our scattering experiments we show that application of the magnetic field to the paramagnetic nanoparticles results in ordered crystal structure formation. Moreover, the crystal structure and lattice parameter changes with the magnetic field strength and demonstrate a phase transition.

We established synthesis of highly monodispersed iron oxide nanoparticles
of different size grafted with polymer and use them to control the self-assembly of nanocomposite varying external parameters: temperature, magnetic field strength and mechanical stress.

Primary authors: KRUTEVA, Margarita; FOKINA, Vladislava; Dr DULLE, Martin (Forschungszentrum Juelich); FÖRSTER, Stephan (Forschungszentrum Jülich)

Presenter: FOKINA, Vladislava

Session Classification: Poster Session II

Track Classification: Soft Matter

Contribution ID: **133** Type: **Talk**

Single-crystal Neutron-diffraction of Ta-substituted and Ga-doped Li7La3Zr2O12 garnet-type solid-state electrolyte material.

Large single crystals of garnet-type Li6La3ZrTaO12 (LLZTO) and Ga-doped Li7La3Ze2O12 (Ga-LLZO) were grown by the Czochralski method and analysed using neutron diffraction between 2.5 and 873 K in order to fully characterize the Li-atom distribution, and possible Li ion mobility in this class of potential candidates for solid state electrolyte battery material. The LLZTO retains its cubic symmetry, with space group Ia-3d,over the complete temperature range. When compared to the other sites, the octahedral sites behave as the most rigid unit and show the smallest increase in thermal parameters and bond length. The La- and Li-sites show mutually similar thermal expansion in their bond lengths up temperature, and the anisotropic and equivalent atomic displacement parameters exhibit a distinctly larger increase at temperatures above 400 K. Detailed inspection of nuclear densities at the Li1 site reveal a small but significant displacement from the 24d to the typical 96h position, which, however, cannot be resolved in the single crystal X-ray diffraction data. The site occupation of LiI ions on Li1 and Li2 remains constant, so there is no change in site occupation with temperature. For Ga-LLZO a phase transition from I-43d to Ia-3d could be identified.

Primary authors: REDHAMMER, Günther (Universität Salzburg); MEVEN, Martin (RWTH Aachen University, Institute of Crystallography - Outstation at MLZ); Mr TIPPELT, Gerold (University of Salzburg); Prof. RETTENWANDER, Daniel (NTNU Trondheim)

Presenter: REDHAMMER, Günther (Universität Salzburg)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **134** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: MÄRKISCH, Bastian (Physik-Department, TUM)

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **135** Type: **Talk**

CLOSED SESSION: PERC Collaboration Meeting

Tuesday, December 7, 2021 4:40 PM (50 minutes)

Presenter: MÄRKISCH, Bastian (Physik-Department, TUM)

Session Classification: Nuclear, Particle, and Astrophysics

Track Classification: Nuclear, Particle, and Astrophysics

Contribution ID: **136** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: GILLES, Ralph

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **137** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: LINK, Peter

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **138** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: GEORGII, Robert

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **139** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: FRIELINGHAUS, Henrich (JCNS)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **140** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: SENYSHYN, Anatoliy

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **141** Type: **Talk**

Welcome

Tuesday, December 7, 2021 9:00 AM (5 minutes)

Presenter: HUGENSCHMIDT, Christoph

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **142** Type: **Plenary talk**

How Neutrons Help Understanding the Behavior of Adaptive Microgels

Wednesday, December 8, 2021 9:30 AM (45 minutes)

Microgels are macromolecular networks swollen by the solvent they are dissolved in. They are unique systems that are distinctly different from common colloids, such as, e.g., rigid nanoparticles, flexible macromolecules, micelles or vesicles. When swollen, they are soft and have a fuzzy surface with dangling chains and the presence of cross-links provides structural integrity - in contrast to linear and (hyper-) branched polymers. Finally, microgels reveal interface activity without being amphiphilic. Due their properties, microgels can be used to tune the particle-to-polymer transition. We will discuss properties of stimuli-sensitive microgels of different architecture (as e.g. ultra-low crosslinked, hollow, multi-shell, anisotropic) in solution. The structure of microgels is investigated by means of scattering methods, especially exploiting the technique of contrast variation in small angle neutron scattering. We will discuss properties of individual microgels as well as the effect of crowding in dense solutions and we compare experimental results to computer simulations.

Scotti, A. et al. Phys. Rev. E 2021, 103, 022612.
Nickel, A. C.; et al. Nano Letters 2019, 19, 8161.
Schmid, A. J.; et al. Scientific Reports 2016, 6, 22736.
Maccarrone, S.et al. Macromolecules 2014, 47, 5982.

Primary author: RICHTERING, Walter (RWTH Aachen)

Presenter: RICHTERING, Walter (RWTH Aachen)

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **143** Type: **Plenary talk**

Closing by the MLZ User Committee

Wednesday, December 8, 2021 4:45 PM (15 minutes)

Presenter: NYLANDER, Tommy (Lund University)

Session Classification: Plenary

Contribution ID: **145** Type: **Plenary talk**

Water dynamics, polymer structure and relaxation in desalination membranes

Wednesday, December 8, 2021 1:15 PM (45 minutes)

Highly crosslinked polyamide (PA) membranes are extensively used in water purification and desalination by reverse osmosis (RO). The talk will present an overview of our recent work on the structure and dynamics of PA membranes, with a combination of neutron and X-ray reflectivity, and neutron spectroscopy. The membranes were synthesised by established interfacial polymerisation routes of m-phenylenediamine (MPD) and trimesoyl chloride (TMC), with prescribed reaction time, concentration and stoichiometry, in both smooth nanofilm and crumpled morphologies. We investigate the dynamics of both polymer network and water using quasi- and inelastic neutron scattering (QENS/INS), exploiting contrast variation and vapour hydration to isolate the dynamics of confined water dynamics. Water is observed to undergo several translational diffusive processes which are examined and quantified for the first time. This multimodal water diffusion is compatible with molecular dynamics simulations and transport models of water through membranes, and permits the estimation of RO performance in water desalination via descriptive engineering models.

Primary authors: Dr FOGLIA, Fabrizia (Imperial College London, University College London); Dr BERNHARD, Frick (Institut Laue Langevin); Prof. ALEXANDRA, Porter (Imperial College London); Prof. LIVINGSTON, Andrew (Imperial College London); Prof. CABRAL, Joao (Imperial College London)

Presenter: Prof. CABRAL, Joao (Imperial College London)

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **146** Type: **Plenary talk**

MLZ – Status and Perspectives

Wednesday, December 8, 2021 9:00 AM (30 minutes)

Presenters: MÜLLER, Martin (Helmholtz-Zentrum Geesthacht); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Session Classification: Plenary

Contribution ID: **147** Type: **Talk**

On the nature of critical compositions of Na0.5Bi0.5TiO3-based lead-free piezoelectrics

Tuesday, December 7, 2021 2:05 PM (25 minutes)

The structural complexities in the Na0.5Bi0.5TiO3 (NBT)-based Pb-free piezoelectrics pose significant challenge regarding understanding of the structure-property correlation. While the critical compositions exhibiting maximum weak-signal piezoelectric response is generally associated to an inter-ferroelectric instability, a combined neutron diffraction and piezoelectric study on three NBT-based systems namely Na0.5Bi0.5TiO3 -BaTiO3, Na0.5Bi0.5TiO3 – K0.5Bi0.5TiO3 and Na0.5Bi0.5TiO3 -SrTiO3 revealed that the maximum piezoelectric response is determined primarily by an in-phase tilt disorder in these systems and not by the inter-ferroelectric instability.

Primary author: Prof. RANJAN, Rajeev (Indian Institute of Science Bangalore. India)

Co-authors: Mr DAS ADHIKARY, Gobinda (Indian Institute of Science, Bangalore); SENYSHYN, Anatoliy

Presenter: Prof. RANJAN, Rajeev (Indian Institute of Science Bangalore. India)

Session Classification: Structure Research

Track Classification: Structure Research