MLZ User Meeting 2022

Report of Contributions

https://indico.frm2.tum.de/e/um22

Contribution ID: **1** Type: **Talk (20 min + 5 min discussion)**

Materials informatics approach on neutron scattering data for the development of anion exchange membranes used for next-generation energy devices

Thursday, December 8, 2022 3:25 PM (25 minutes)

We aim to apply "materials informatics"(MI) for the development of high-performance anion-exchange membranes (AEM), which may be applied to next generation energy devices, such as non-platinum fuel cell hybrid vehicles and all solid secondary batteries. Currently, there are two major obstacles to using MI for such systems: the unclear higher-order (hierarchical) structure/function relationship of AEM and the lack of a comprehensive structural database under various practical temperature/humidity conditions. We plan to use scattering and simulation methods, in particular the unique CV-SANS (Contrast-Variation Small Angle Neutron Scattering) technique with precise Partial Scattering Function (PSF) analysis, to obtain an accurate structure of each component in real AEMs under practical operating conditions and also to target various AEMs prepared by Radiation Graft Polymerization (RGP), which allows to impart new functionality to graft polymers while maintaining the mechanical and thermal properties of base polymers. A structural dataset will be defined through CV-SANS, microscopy and simulations, and we aim to create new optimized AEM through machine learning algorithms using this database. In our recent studies on hydrated proton exchange membrane (PEM) systems we introduce CV method to conventional SANS measurements to give multiple profiles for one sample under one operation condition (i.e. multiple equations), which are necessary for unique PSF analysis to determine precise structure of each component [1, 2]. Examples of PSF analysis of CV-SANS data collected at KWS-2 SANS instrument and the plans on using MI for next generation AEMs will be reported.

[1] Y. Zhao et al., Macromolecules 54, 4128 (2021).
[2] Y. Zhao et al., Macromolecules in press (2022).

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Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **2** Type: **Talk (20 min + 5 min discussion)**

Neutrons and X-ray methods for investigation of Li-ion batteries at material, electrode and cell level

Thursday, December 8, 2022 3:50 PM (25 minutes)

Neutrons are powerful and have unique characteristics, which make possible non-destructive and operando characterizations of cylindrical and prismatic Li-ion batteries. X-rays are an equally competent tool that can provide complementary information on pouch type Li-ion cells during cell operation. Expectedly, both are also capable of providing information at material and electrode level. This contribution will show with several examples how neutrons and x-rays methods such as diffraction, small and wide-angle scattering and neutron depth profiling were helpful in estimating electrochemically active Li losses, Li plating and Li diffusion kinetics at cell level, Li distribution profiles and pore morphologies at electrode level, interplay between mechanics and their molecular origins at material level. These insights are useful to understand the improvement in cell performance by (a) altering the graphite electrode morphology, (b) by preparing composite silicon-graphite electrodes, (c) by Si deposition on TiO2 nanotubes, (d) and by applying polymer coatings to Li metal anode surfaces.

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Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **3** Type: **Poster**

The new data evaluation group for the MLZ User community

Friday, December 9, 2022 2:00 PM (3 hours)

Getting beamtime at MLZ and performing experiments for the first time is an exhilarating experience. For some new users, however, data analysis of acquired data is quite challenging. To avoid situations where valuable data is left untreated due to lack of experience and adequate support, MLZ creates a new group for user support, which will work in close cooperation with the instrument scientists.

The data evaluation group is a team of scientists, who have several years of technical and scientific work experience at selected neutron and X-ray instruments at the MLZ and in using various software packages for evaluation of the obtained neutron and X-ray data. The goal of this newly established group is to offer guidance and active support to the user community, particularly to new users, in both data evaluation and reduction steps, and to assist them in obtaining meaningful insights from obtained data by offering also writing support for preparing a publication.

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Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **4** Type: **Poster**

The optimized thermal beamport SR8 at the research neutron source Heinz Maier-Leibnitz

Friday, December 9, 2022 2:00 PM (3 hours)

The neutron powder diffractometer SPODI is one of the most active instruments at the research neutron source Heinz Maier-Leibnitz. However, the demands of the user community far exceed the available beam time. Therefore, the thermal beamport SR8 will be optimized to allow the simultaneous operation of the three powder diffractometers SPODI, FIREPOD and ERWIN. Due to the unique characteristics of the three instruments, which will be presented in detail, they will be able to cater for a wide range of experimental demands.

SPODI is going to remain the high-resolution option in this suite of instruments. Due to neutron guides with optimized geometries, SPODI will feature a 20% increase of the neutron flux, while retaining its flat resolution curve with typical small FWHMs of below 0.35°. Careful Monte-Carlo simulations show that the neutrons transmitted through the SPODI monochromator can be efficiently re-utilized by the powder diffractometer FIREPOD in simultaneous operation.

With a planned neutron flux of 2*10^7 n/s cm^2 –one order of magnitude more than SPODI –and its eight large area detectors, FIREPOD will be a dedicated high throughput instrument, ideally suited for a broad range of fast parametric studies. Finally, ERWIN will complement the current single crystal option RESI. It is characterized by a large curved 2D detector with a virtually seamless coverage of ~135° and a choice of three different monochromators allowing for a broad range of usable wavelengths.

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Presenter: HAUF, Christoph

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **5** Type: **Poster**

Silicon detector for neutron beta decay measurements with PERC

Friday, December 9, 2022 4:35 PM (25 minutes)

The PERC facility is currently under construction at the FRM II in Garching, Germany. 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 to minimize 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.

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Presenter: LEBERT, Manuel (Technical University Munich)

Session Classification: Poster Session

Track Classification: Nuclear, Particle and Astrophysics

Contribution ID: **6** Type: **Talk (20 min + 5 min discussion)**

Architectural dynamics of photosynthetic thylakoid membranes during simulated coral bleaching

Thursday, December 8, 2022 3:00 PM (25 minutes)

Corals bleach under a number of stresses, one of these being thermal stresses exemplified by the 2010, 2016 and 2017 bleaching events in Australia's Great Barrier Reef. Such events demand detailed physiological understanding in order to provide predictive knowledge of the effects of rising ocean temperatures on coral. One technique suitable for in situ examination of the effect of thermal stresses on corals, and in particular of the intra-cellular membranes associated with the photosynthetic apparatus of the symbiotic algae, known as zooxanthellae or Symbiodinium living in hospice in coral cells is small angle neutron scattering (SANS).(Jakubauskas et al., 2019) When applied to photosynthetic organisms such as cyanobateria the method can provide a statistical and non-destructive perspective on the organisation of photosynthetic membranes. Here we report the temperature induced changes of photosynthetic membranes in Symbodium living within individual Aiptasia anemone specimens extracted from SANS data using a model of the structure. The results provide a simple perspective on the effects of temperature on the photosynthetic machinery of the symbiote.

Jakubauskas, D., Ł. Kowalewska, A. V. Sokolova, C. J. Garvey, K. Mortensen, P. E. Jensen, and J. J. K. Kirkensgaard. 2019. Ultrastructural modeling of small angle scattering from photosynthetic membranes. Scientific Reports 9(1):19405.

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Presenter: GARVEY, Christopher (MLZ)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **7** Type: **Talk (20 min + 5 min discussion)**

Hydration Water Dynamics in a Thermoresponsive Polymer Solution Under Pressure

Thursday, December 8, 2022 1:40 PM (25 minutes)

The water dynamics is key to functionality and phase behavior of synthetic and biological polymers. Responsive polymers react strongly to external stimuli such as temperature and pressure triggering chain collapse and phase separation. We investigate the dynamic behavior of hydration water in a 25 wt% aqueous poly(*N*-isopropyl acrylamide) (PNIPAM) solution in dependence on temperature (25 −50 ℃) and pressure (0.1 −130 MPa) employing quasi-elastic neutron scattering (QENS) at TOFTOF [1]. The susceptibility spectra reveal the relaxation peak of the hydration water near 10 GHz, in addition to the known dynamic processes of bulk water. At atmospheric pressure, the relative population of (bound) hydration water sharply decreases upon heating from the one-phase to the two-phase state, i.e. the chains dehydrate strongly at their coil-to-globule transition. In contrast, at 130 MPa, no sharp decrease is observed, i.e. the dehydration takes place over a much broader temperature range, in consistency with recent molecular dynamics simulations [2]. This suggests an enhanced hydrophobic hydration at high pressure. Using perdeuterated PNIPAM along with QENS at TOFTOF and SPHERES allowed us to suppress the signal of the chain segments and to identify and characterize the behavior of the different types of bound water at the transition.

1. B.-J. Niebuur, A. Schulte, C. M. Papadakis et al., Macromolecules 2019, 52, 1942.
2. L. Tavagnacco et al., Phys. Chem. Chem. Phys. 2021, 23, 5984.

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Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **8** Type: **Poster**

The backscatter detector system of PERC

Friday, December 9, 2022 3:30 PM (1h 30m)

The PERC facility is currently under construction at the FRM II. It aims to measure the beta spectrum of neutron decay more precisely than its predecessors PERKEO II and PERKEO III, enabling the determination of several correlation coefficients in neutron decay with an improved precision by one order of magnitude. Of particular interest is the so-called beta asymmetry parameter A. PERC aims to measure A with an unprecedented precision of $A = 5 \times 10^{-5}$ making it possible to determine the CKM matrix element V_{ud} most precisely and test the unitarity of the CKM matrix. PERC will observe neutron decay in an 8 m long neutron guide and a high magnetic field will guide the charged decay products downstream to the main detector. To achieve the targeted precision, we have to identify backscattering events, in which the electron only deposits a part of its energy in the detector, as this would otherwise alter the spectrum. The magnetic field guides backscattered electrons downstream, where a detector system will identify these events by the coincidence time. The backscatter detectors will consist of two scintillation detectors and SiPM arrays on the backside for readout. Due to the high background in that area, spatial resolution is necessary to avoid accidental coincidences. Using the simulation tool Geant4 I compare different possible setups in their energy and spatial resolution. I present the results of these simulations and the status of the development of the detectors.

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Presenter: BERNERT, Karina (TUM)

Session Classification: Poster Session

Track Classification: Nuclear, Particle and Astrophysics

Contribution ID: **9** Type: **Talk (20 min + 5 min discussion)**

Neutron coating development applied to non-depolarizing Cu/Ti supermirrors

Thursday, December 8, 2022 1:40 PM (25 minutes)

In the last two years the neutron optics group of FRM II has successfully sputtered non-depolarizing m=2 Cu/Ti supermirrors, which have been prepared with a standard DC magnetron sputtering facility. Control on the roughness grow and interdiffusion allowed us to get a very good maximum angle of total reflection (ca. 0.21°/λ) and polarized neutron reflectivity above 90%, as measured at the instrument GINA, located at BNC in Budapest.

The magnetic behavior of the Cu/Ti coating was checked by means of SQUID measurements at the WMI in Garching to be slightly ferromagnetic with magnetic moment of 10E-3 Bohr-magneton/atom. For comparison, Ni/Ti and Ni(Mo)/Ti supermirrors were also measured, finding magnetizations of 0.55 Bohr-magneton/atom for Ni and 0.11 Bohr-magneton/atom for Ni(Mo), in agreement with data found in the literature.

By knowing the structure of the sample, the simulation programs GenX and SimulReflec were used to distribute the magnetization measured by SQUID along the whole supermirror structure in order to check which would be the theoretical Spin Flip Reflectivity (i.e. depolarization) that this magnetization would deliver, finding a maximum value of a few times 10E-6.

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Session Classification: Nuclear, Particle and Astrophysics

Track Classification: Nuclear, Particle and Astrophysics

Contribution ID: **10** Type: **Poster**

Laterally Resolved Neutron Depth Profiling with the N4DP Instrument

Friday, December 9, 2022 3:30 PM (1h 30m)

Neutron Depth Profiling (NDP) is a non-destructive, element-specific, high-resolution nuclear analytical technique, which is often used to probe concentration profiles of lithium, boron, nitrogen, helium and several other light elements in different host materials. The N4DP instrument is located at the Prompt Gamma Activation Analysis (PGAA) beam line of Heinz Maier-Leibnitz Zentrum (MLZ), which provides a cold neutron flux up to $5 \times 10^{10}\,\mathrm{s}^{-1}\mathrm{cm}^{-2}$.

We applied NDP to study the lithium-ion concentration gradient in energy storage systems, e.g. Li-ion batteries. Here, NDP reveals the evolution of immobilized lithium, which is one of the main causes of battery lifetime limitation. Furthermore, the status of the ongoing development towards 4D profiling is presented, where not only the concentration gradient, but also the lateral position of probes as well as its time evolution will be measured. For this, a highly segmented Si-based detector with 32×266 stripes, including integrated, self-triggering electronics, were successfully assessed. Using a camera-obscura geometry setup, we aim for lateral scanning with a space resolutions down to 100 μm × 100 μm and highest time resolutions using a newly developed elliptical focusing neutron guide. This project is supported by the BMBF, Contract No. 05K16WO1, 05K19WO8.

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Presenter: NEAGU, Robert

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **11** Type: **Poster**

Texture and microstructure evolution of TNM alloy during hot compression

Friday, December 9, 2022 3:30 PM (1h 30m)

Owing to low density (3.8-4.0g/cm3), high specific strength and stiffness, excellent creep resistance, and good corrosion resistance, the β-solidifying TNM alloys with properly aligned (α2+γ) lamellar structure have been considered as excellent candidates for modern turbine blades. Recently, it has been evidenced that when the γ lamellae are oriented to the load direction the mechanical properties of the alloys can be greatly increased, thus, lamella orientation control has become an interesting topic for property optimization.
In the present work, the microstructure and texture of a TNM alloy (Ti-43Al-4Nb-1Mo-0.1B (at%) hot compressed to different strains at various strain rates were characterized by synchrotron radiation diffraction at a macroscopic scale to obtain the bulk texture information and by SEM EBSD at mesoscopic scale to analyze with respect to the orientation relationships and microstructure. After the uniaxial compressive hot deformation at 1280℃ to different deformations at different strain rates, it seems that the microstructure changed and the α to lamellar (α+γ) was inhibited with the increase of the strain rate. The microstructure became mainly composed of the alpha phase. All three phases can be textured.
In conclusion, texturization of the TNM alloy seems to be possible thanks to the hot compression. It leads to different types of microstructures depending on the amount of deformation and the strain rates as well as the used temperature.

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Presenter: KEITA, Mohamed

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **12** Type: **Talk (20 min + 5 min discussion)**

Magnetic excitations in long-range stripes of Pr2NiO4+δ

Thursday, December 8, 2022 3:50 PM (25 minutes)

Magnetic excitations in stripe-phases of $La-$based hole-doped $214-$ nickelates, especially in the $Sr-$doped ones, have been vigorously explored using inelastic neutron scattering (INS) studies. In $Sr-$ doped samples, the spin stripe correlation is relatively short-ranged due to unavoidable disorder introduced by the randomly distributed dopant. However, often the results have been compared with the linear spin wave (LSW) theory-based calculations, which assume long-range spin-stripe ordering.

In this talk, we will present the effect of long-range spin stripe ordering on the magnetic excitations of an $O-$ doped $214-$ nickelate Pr_2NiO_{4+} ($\delta \sim 0.24$), where we find the spin stripe correlation is quite long-ranged ($\sim$ 50 Å) compared to the $Sr-$ doped $Pr_{2-x}SrNiO_4$ ($\sim$ 20 Å). For our investigation, we have performed the INS measurements using the thermal triple-axis spectrometer PUMA at MLZ, IN8 at ILL, and time-of-fight spectrometer MAPS at ISIS. Our investigation presents an intriguing observation of multiple equivalent weak modes in the spin wave dispersion of $O-$ doped $Pr_{2-x}SrNiO_4$ [1], which we have interpreted from the internal periodicity of the long-range ordered discommensurated spin stripes.

Reference: [1] A. Maity, R. Dutta, A. Marsicano, A Piovano, J. Ross Stewart and W. Paulus Phys. Rev. B 103, L100401 (2021).

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Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

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

Novel type polarization analysis using multi-analyzer setup at PUMA

Friday, December 9, 2022 3:30 PM (1h 30m)

The thermal triple-axis-spectrometer PUMA at the neutron research reactor FRM-II (MLZ) is one of the most robust, and yet extremely flexible instruments worldwide of its kind. In addition to the "*normal triple axis*"setup, PUMA delivers a good number of unique features to meet the ever-growing demands of the scientific community worldwide. Multiplexing, using the multi-analyzer and multi-detector systems is one of them, which consists of eleven arbitrarily configurable analyzer-detector channels. In particular, single-shot kinetic experiments are well suited as the setup allows the realization of an entire $(Q,)$-scan within a time scale even less than a minute as a
function of any external stimulant. Moreover, the same setup can be used for polarization experiments very efficiently. By directing the spatially separated different spin-states of the scattered neutrons into the different analyzer channels, the spin-flip (SF) and the non-spin flip (NSF) components can be simultaneously determined [1,2]. Especially in the case of kinetic time-resolved experiments, where both spin states need to be registered synchronously at the same state of the sample, this setup is of absolute necessity. In this talk, I will report on the details of the current status of polarization analysis setup at PUMA and present results from the pilot experiments.

References: [1] S. Schwesig et al., A 877 (2018) 124–130. [2] A. Maity at al., Physica Status Solidi B 257, 1900704 (2020).

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Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **14** Type: **Talk (20 min + 5 min discussion)**

Scaling and Fouling in Reverse Osmosis Wastewater Desalination –Operando Studies with Small-Angle Neutron Scattering

Thursday, December 8, 2022 3:50 PM (25 minutes)

We present operando small-angle neutron scattering (SANS) experiments on silica and protein (BSA) fouling as well as scaling from a simulated secondary effluent (SSE) at the surface of a polyamide RO membrane at close to realistic conditions. In the first part we present a study of aqueous silica dispersions combining the parameters of colloidal radius, volume fraction, and ionic strength. The observation of Bragg diffraction representing a crystalline cake layer of simple cubic lattice structure is observed. Cake layer formation proved to be a reversible process, which could be removed again at larger cross-flow. Only in one case we observed an irreversible cake layer formation showing the characteristics of an unstable phase transition of otherwise liquid-solid phase transitions of first order. The second part deals with organic fouling of BSA dissolved in the SSE solution. Mixing 1 g/L BSA to SSE leads to an instantaneous formation of stable organic-mineral colloids, i.e. composite particles of about 1 size only increasing in number density. Their composition was about 50% protein and 50% mineral, mainly calcium phosphate and carbonate as analysed from former contrast variation SANS measurements. After about 17 h the particle size increases to about 3 without any external influence and showing no effect on permeate flux and electric conductivity. Similar behavior was already observed in former in vitro experiments.

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Presenter: Dr SCHWAHN, Dietmar (JCNS)

Session Classification: Soft Matter

Track Classification: Soft Matter

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

REFSANS: The horizontal time-of-flight reflectometer with GISANS option at the Heinz Maier-Leibnitz Zentrum

Friday, December 9, 2022 3:30 PM (1h 30m)

REFSANS is the horizontal TOF reflectometer at the MLZ, designed to enable reflectometry and GISANS studies of any interface, as well as to give simultaneous access to a range of Qz values, which is especially useful to study air-liquid interfaces or kinetic phenomena.
Wavelength resolution may be tuned from 0.2 % up to 10%. The optics comprises neutron guide elements with different channels and special apertures to provide, on the one hand, slit smeared beams for conventional reflectometry and, on the other hand, point focused beams for GISANS measurements. Furthermore, it is possible to independently control the horizontal and vertical beam divergence, in dependence on the sample characteristics.
The investigation of kinetic processes is possible thanks to the possibility to embrace a Qz-range with a single instrumental setting. Time resolution can be pushed down to 30 s with data recorded in event-mode: this feature makes possible to perform various time re-binnings in order to tune the resolution/ intensity trade-off after the experiment. Beside the typical sample environment, the realization of an electrochemical compact cell and the design of a humidity cell are in progress, in order to allow the investigations of electrode processes and of processes in a controlled atmosphere. Furthermore, simulations to realize a flexible focusing optical system are in progress, capable of offering unique possibilities for the investigations of small samples ($\leq 20 \cdot 20$ mm^2).

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Presenter: MANGIAPIA, Gaetano

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **16** Type: **Talk (20 min + 5 min discussion)**

Innovative approaches to beam monitoring.

Thursday, December 8, 2022 5:35 PM (25 minutes)

Optimization of the shape and intensity of a positron beam requires suitable beam diagnostics. The speed with which a low-energy positron beam can be optimized prior to a measurement is presently limited by available detection techniques, resulting in a sizeable loss of beam time to optimization. In this talk we will present two novel approaches to the detection of the position, shape and intensity of a low energy positron beam which our collaboration has been investigating in the past two years.

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

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **17** Type: **Poster**

Tuning of protein adsorption on nanoparticles using oppositely charged surfactant and multi-valent ions

Friday, December 9, 2022 3:30 PM (1h 30m)

The integration of the nanoparticles with proteins has a prime interest in the field of nanobiotechnology where these complexes are aimed to be utilized in different applications such as targeted drug delivery, biosensing, etc. [1]. The protein adsorption on nanoparticles is governed by several interactions such as hydrogen bonding, electrostatic complexion, hydrophobic attraction, etc. Herein, the interaction of cationic lysozyme protein with the anionic Ludox HS40 silica nanoparticle has been tuned by anionic SDS and multi-valent ZrCl4 ions in the three-component systems. The unique advantage of contrast matching SANS (bulk contrast, micelle contrast, and nanoparticle contrast) has been utilized to probe the role of individual components in the three-components system [2]. The results demonstrate that selective additive induced preferential binding of the protein (lysozyme-SDS/lysozyme-HS40 nanoparticles) and the multivalent ions driven charge inversion of the nanoparticles/proteins can be utilized to create switching between the protein adsorption and non-adsorption. These parameters can also enable the control over the undesired protein adsorption and nanoparticle aggregation in the nanoparticle-protein systems [3].

References

1. M. Hadjidemetriou et al. Nat. Nanotechnol. 12, 288 (2017).
2. D. Saha et al. Soft Matter 18, 434 (2022).
3. S. Kumar et al. Appl. Phys. Lett. 118, 153701 (2021).

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Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **18** Type: **Talk (20 min + 5 min discussion)**

Thin film fabrication for neutron investigations

Thursday, December 8, 2022 5:35 PM (25 minutes)

The Jülich Centre for Neutron Science offers the opportunity to fabricate thin film samples by Molecular Beam Epitaxy (MBE). We are running an MBE setup 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! In the past, we have produced simple Fe layers, complicated multilayers consisting e.g. of layers of Ti, Pt and Co, transition metal oxides like $La_{0.7}Sr_{0.3}MnO_3$ or oxides like TiO2.

Discuss your ideas with the thin film lab staff at the poster and then write the proposal! There are two options for access: In remote access the thin film lab staff fabricates the sample for you and in collaborative access you fabricate the sample with support by the thin film lab staff. Evidently, the first option only works if the growth parameters are well known.

The samples can be investigated in-situ by reflection high and low energy electron diffraction for surface structure analysis while Auger electron spectroscopy may be applied for in-situ chemical surface analysis.

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

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

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **19** Type: **Poster**

Pt/gCN loaded hydrogel films as a H2 production device

Friday, December 9, 2022 4:35 PM (25 minutes)

Photocatalysis of water is becoming one of the pillars of green approaches to obtain sustainable energy supply. The water splitting reaction is an easy way to implement the sun to produce hydrogen-based energy. Pt loaded graphitic carbon nitride (g-CN) has been found as a promising candidate for the H2 evolution reaction under visible light. It showed a high H2 evolution efficiency in aqueous solution despite the photocatalyst spreading in solution. Previous works proposed to introduce hydrogels as host matrix and water storage for the water splitting reaction. This work aims to develop this system in a polymer thin film configuration to make it suitable for industrial purposes. Poly(N-isopropylacrylamide) (PNIPAM) thin films exhibit good swelling capacity in water vapor atmosphere and appear suitable for a hybrid thin film system. A new isomer poly(N-vinylisobutyramide) (PNVIBAM) has also been proposed due to its higher lower critical solution temperature (LCST) in aqueous solution (≈39℃), which makes it more stable in ambient environment. Therefore, an initial comparison of both polymers is based on in situ spectral reflectance and FT-IR measurements. The hybrid thin films have been spray coated to proceed grazing incident small angle x-ray scattering (GISAXS). G-CN/Pt blended polymer films microstructure is analysed under light irradiation conditions and future neutron reflectivity experiments will provide information about the water distribution in the hybrid layers.

Primary author: LE DÛ, Morgan

Co-authors: REITENBACH, Julija; REUS, Manuel (TUM E13); SUN, Kun; LI, ZERUI (TUM); Dr BERNSTORFF, Sigrid (Elettra-Sincrotrone Trieste S.C.p.A.); HENSCHEL, Cristine (Fraunhofer-Institut für Angewandte Polymerforschung); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie); Prof. LASCHEWSKY, André (Fraunhofer-Institut für Angewandte Polymerforschung); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: LE DÛ, Morgan

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **20** Type: **Poster**

Precise Measurements of the Decay of Free Neutrons

Friday, December 9, 2022 4:35 PM (25 minutes)

We review the impact of new and highly precise neutron beta decay data with a focus on recent results from neutron lifetime, beta asymmetry, and electron-neutrino correlation experiments. From these results, we extract weak interaction parameters with unprecedented precision. This is enabled also by progress in effective field theory and lattice quantum chromodynamics. Limits on New Physics beyond the Standard Model of particle physics derived from neutron decay data are sharper than the corresponding limits derived from high-energy experiments. Recent experimental results allow an extraction of the element V_{ud} of the Cabibbo-Kobayashi-Maskawa matrix with very competitive precision to superallowed nuclear beta decays and confirm the currently prominent Cabibbo-angle anomaly.

We discuss the prospects and impact of the upcoming neutron beta decay experiment PERC at the MLZ, and present its status.

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

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

Session Classification: Poster Session

Track Classification: Nuclear, Particle and Astrophysics

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

Antisite Li\Ni disorder in the NCA-type battery cathode

Friday, December 9, 2022 3:30 PM (1h 30m)

The electrochemical efficiency of Li-ion batteries is largely determined by the diffusivity of Li ions and the transport of electrons between electrode materials in the cell. In nickel-containing cathode materials the mixed Li\Ni occupations often occurs, leading to structural disorder, blocking of the 2D diffusion pathways of Li^{+} by Ni^{2+}, as well as the reduction of the capacity and structure stability. Mixed transition metal batteries like Li(Ni,Co,Al)O_2 and high nickel content Li(Ni,Mn,Co)O_2 are considered to be promising cathode materials showing better cycling stabilities, lower toxicity, lower costs etc. and are therefore of particular interest from the viewpoint of Li\Ni disorder [1, 2]. In literature, the studies and understanding of factors causing cation mixing is still controversial and are poorly presented. In the current contribution structural parameters of selected nickel-containing cathodes, obtained by neutron powder diffraction with the instrument SPODI at FRM II will be discussed together with their electrochemical characteristics.
[1] J. Zheng, Y. Ye, T. Liu, Y. Xiao, C. Wang, F. Wang and F. Pan, Ni/Li Disordering in Layered Transition Metal Oxides: Electrochemical Impact, Origin, and Control, Acc. Chem. Res. 52, 2201-2209 (2019).
[2] O. Dolotko, A. Senyshyn, M. J. Mühlbauer, K. Nikolowski and H. Ehrenberg, Understanding structural changes in NMC Li-ion cells by in situ neutron diffraction, Journal of Power Sources 225, 197-203 (2014).

Primary author: HÖLDERLE, Tobias

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

Presenter: HÖLDERLE, Tobias

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **22** Type: **Talk (20 min + 5 min discussion)**

Aging-related changes in the Lithium Distribution of 18650-type Li-ion batteries

Thursday, December 8, 2022 5:35 PM (25 minutes)

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 previous studies it was shown that with cell aging the distribution of the lithium-ions in the graphite anode of 18650-type lithium-ion batteries changes [3]. In this contribution, a set of cells at different state-of-health was measured with spatially resolved neutron powder diffraction. The results have shown changes of the lithium distribution over the lifetime of a commercial 18650-type lithium-ion battery.

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.
3. Mühlbauer, M.J., et al., Inhomogeneous distribution of lithium and electrolyte in aged Li-ion cylindrical cells. Journal of Power Sources, 2020. 475: p. 228690.

Primary author: PETZ, Dominik

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

Presenter: PETZ, Dominik

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **23** Type: **Poster**

Understanding the Lithium Depth Profile Upon Lithiation of Extracted Silicon-Based Anodes

Friday, December 9, 2022 4:35 PM (25 minutes)

A prominent strategy to increase the capacity of Lithium Ion Batteries is the use of silicon as anode material. However, the volumetric increase of silicon upon lithiation regularly results in a low cycling stability of the material. Our strategy is based on a partial lithiation of silicon to ~30%, which leads to a significant gain in cycling stability while maintaining a high capacity. The knowledge of the lithium distribution across such silicon electrodes is crucial to assess their behavior in working cells. In our study, we use Neutron Depth Profiling (NDP) on extracted silicon-based anodes to reveal the lithium depth distribution after different formation and lithiation steps. Thereby, we investigated three states of charge (SOC) and the formation with and without $LiNO_3$ as electrolyte additive, which can significantly increase the cycling stability of silicon. Our results show that lithium is evenly distributed in depth across all studied electrodes. The formation already leads to a lithium concentration of ~9mol/cm^2, which is inferred to be a consequence of lithium which is irreversibly bound in the as-formed solid-electrolyte-interface (SEI). With increasing SOC (15%, 30%) the lithium concentration consistently increases. Also, we observe a significant swelling of the electrode during the lithiation process. Notably, the $LiNO_3$ electrolyte additive leads to a higher lithium content in the SEI, which is a first indicator of differences in the formation process.

Primary author: GROSSMANN, Lukas

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

Presenter: GROSSMANN, Lukas

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **24** Type: **Poster**

Relocation of the cold triple axis spectrometer FLEXX to MLZ, Munich: Larmor diffraction and inelastic scattering

Friday, December 9, 2022 3:30 PM (1h 30m)

The cold triple-axis spectrometer (TAS) FLEXX at HZB is a well-designed and upgraded instrument [1-4]. There is a strong wish that this excellent instrument should be preserved for the community after the shutdown of the HZB neutron source. One attractive gap in the present instrumentation suite of MLZ, is the Larmor-diffraction technique (LD) and, as a natural extension, cold neutron resonant spin echo (NRSE). LD permits the exact measurement of lattice constants and their distribution (internal strains, structural distortions or magnetostriction). In addition, spin correlation lengths in antiferromagnets and antiferromagnetic domain sizes of up to 1 μm can be determined. For looking at time-dependent processes one needs the NRSE mode. TAS comes at no extra cost, as is the main backbone of such an instrument.
The instrument will be placed on a cold neutron source. This will allow for a x4 increase in Q resolution, as well as most importantly access to the low Q region, as compared to the existing TRISP@MLZ. Further, new developments are under way to allow for application of magnetic fields at the sample, hitherto not possible. This opens up new vistas in the exploration of materials. A last attractive option is the possibility to combine high magnetic fields together with cold TAS.

[1] M. Skoulatos et al., NIMA 647, 100 (2011).
[2] M.D. Le et al., NIMA 729, 220 (2013).
[3] F. Groitl et al., Rev. Sci. Instrum. 86 025110 (2015).
[4] K. Habicht et al., EPJ 83, 03007 (2015).

Primary authors: SKOULATOS, Markos (TUM); HERTWIG, Martin; GEORGII, Robert; KELLER, Thomas (MPI for Solid State Research, Stuttgart)

Presenter: SKOULATOS, Markos (TUM)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

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

Friday, December 9, 2022 3:30 PM (1h 30m)

Organic semiconductors have attracted intense attention due to their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, poly(3,4-ethylene dioxythiophene):poly(styrenesulfonate)(PEDOT:PSS) is the most studied conducting polymer system due to its intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility. The combination of DMSO-solvent doping and physical-chemical DMSO/salt de-doping in a sequence has been used to improve the thermoelectric 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 % Na2SO3 in the DMSO/salt mixture (v/v), outperforming 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 author: TU, Suo (Institute of Functional Materials)

Co-author: MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: TU, Suo (Institute of Functional Materials)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **26** Type: **Poster**

Nuclear Analytical Chemistry at the cold neutron beam of MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

The cold neutron beam at MLZ offers unique conditions for nuclear analytical chemistry. The analytical facility accommodates several instruments being under development or recently upgraded. The focusing guide has been replaced with a truly-curved elliptical guide ensuring a more homogeneous beam with a smaller divergence and with coinciding focal points, which serves all instrumental setups much better. Upgraded spectrometers have been employed enabling better Compton suppression, improved timing for coincidence measurement together with list-mode acquisition. These features will be used in new dynamic in-beam activation analytical measurements. Prompt Gamma Activation Analysis (PGAA) is a routine technique used since the reactor start. It exploits the advantages of the strong neutron beam with measuring small samples (with masses less than a mg), or activating them in the nearly parallel cold neutron beam with counting the activity in a dedicated low-background chamber. In-beam activation analysis (ibNAA) proved to be an important addition to PGAA. This technique will be further developed with many repeated irradiation and counting cycles using a transfer system to a low-background position on the top of the PGAA setup. The irradiation and counting times could be as short as 1 s, while the transfer times a few tenths of a second. With cyclic in-beam setup, several hard-to-measure elements, like F, Ag, Pb, even O-19 isotope become available with much better sensitivities.

Primary author: REVAY, Zsolt (PGAA)

Co-author: Dr STIEGHORST, Christian (TUM / FRM II)

Presenter: REVAY, Zsolt (PGAA)

Session Classification: Poster Session

Track Classification: Material Science

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

Photomodulation of the cloud point of thermoresponsive polymers

Friday, December 9, 2022 3:30 PM (1h 30m)

Thermoresponsive copolymers are nowadays useful materials for drug delivery [1]. Incorporating a light sensitive functionality as a second non-invasive stimulus, their lower critical transition temperature (LCST) can be modulated at will, achieving a switching of the conformation and the water solubility by a change of temperature or by irradiation with light. Here, we investigate the effect of content and isomerism of incorporated azobenzene moiety on the cloud point of poly(methoxy diethylene glycol acrylate) and poly(N-ethylene acrylamide). We show a drastic decrease in cloud point for both systems after introduction of azobenzene, and for the first system, the *cis*-form gave an unexpectedly lower cloud point than the *trans*-form, which could be probably explained by the aggregation and loop effect. Further work will be focused on the second system, exploring the phase transition behavior upon the irradiation.

Primary author: ZHANG, Peiran (TUM)

Co-authors: Mr STEINBRECHER, René (University Potsdam); Ms MIASNIKOVA, Anna (University Potsdam); MONTOYA, Adrián Benítez (University Potsdam); LASCHEWSKY, André (University Potsdam); BUSCHBAUM, Peter Müller (Technical University of Munich); PAPADAKIS, Christine M. (Technical University of Munich)

Presenter: ZHANG, Peiran (TUM)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Deuteration Service for Users of the MLZ Neutron Scattering Instruments

Friday, December 9, 2022 3:30 PM (1h 30m)

In order to provide users of the neutron scattering instruments at the MLZ with the appropriate partially or fully deuterated materials the JCNS has started a deuteration service, primarily from our core competence areas of polymers and ethoxylation.

This year we have held our first call for synthesis proposals. During the MLZ user meeting we wish to present some of the results of this call and inform the users about our upcoming calls.

We offer the deuteration of various polymers, surfactants and a variety of small molecules. Recent advances include the synthesis of deuterated thermoresponsive polymers such as PNIPAM and other polymers of the acrylate and methacrylate family. We have also achieved the synthesis of fully deuterated low molecular weight PEGs. Finally, we wish to present the deuteration of various surfactants including TWEEN 20 and different alcohol ethoxylates.

We look forward to talk with users of the MLZ neutron scattering instruments about their needs in terms of deuterated compounds and are also open to discuss longer term cooperation.

Primary authors: ALLGAIER, Jürgen (FZ Jülich); SCHWÄRZER, Kuno

Presenter: SCHWÄRZER, Kuno

Session Classification: Poster Session

Track Classification: Soft Matter

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

Neutron Activation Analysis at MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

Neutron Activation Analysis is still one of the most sensitive trace-element analytical method. FRM II reactor offers unique possibilities for NAA with its high-flux highly thermalized neutron field. The method has been made available in the user system. The reactor is equipped with several irradiation facilities: rabbits, capsule irradiation system and the so-called "fishing line" position enabling the irradiation of materials in a broad mass and time range. Three HPGe detectors equipped with digital spectrometers are currently used for spectrum acquisition in the laboratory of the nearby building of the Radiochemistry Department (RCM). Data evaluation is based on the k0 standardization method and is performed with HyperLab and Kayzero programs. A smart-controlled, list-mode-based acquisition of the gamma-ray spectra, as well as an automated sample changing are planned developments at the NAA instrument.
The scientific applications currently concentrate in the fields of archaeometry, cultural heritage, geology, cosmochemistry (meteorites), biology and food research, as well as recycling technologies. There is a particular demand for developments of new reference materials in archaeometry where NAA is to be used in their certification. FRM II reactor is also ideal for the determination of nuclear data, especially of more precise k0 values serving the needs of nuclear analytical and data communities.

Primary author: Dr STIEGHORST, Christian (TUM / FRM II)

Co-author: REVAY, Zsolt (PGAA)

Presenter: Dr STIEGHORST, Christian (TUM / FRM II)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **30** Type: **Poster**

Tunable morphologies in charged pentablock terpolymers in thin film geometry: effect of solvent vapor annealing

Friday, December 9, 2022 3:30 PM (1h 30m)

Self-assembled morphologies of thin films of a pentablock terpolymer with a symmetric architecture of two types of pH-responsive midblocks and short hydrophobic end blocks are investigated. Different degrees of charge, installed for the two pH-responsive blocks by varying the pH-value of the aqueous solution used for spin-coating, strongly define the film formation behaviour [1]. However, with the high glass transition temperatures of the middle pH-responsive block and the hydrophobic end blocks, the as-prepared films are not necessarily in equilibrium. Here, we investigate further accessible morphologies by swelling the films in the vapors of solvents having different selectivity. In situ grazing-incidence small-angle X-ray scattering (GISAXS) suggests that water vapour (exclusively swelling the pH-responsive blocks) disorders the film in the swollen state, while it leaves the nanodomains rather intact after drying. Methanol vapor (swelling all blocks), in contrast, enhances microphase separation, and the film stays ordered at all stages of SVA. Restructurization, in general, was found to be more pronounced at higher pH-values, where both pH-responsive blocks are uncharged.

[1] F. A. Jung, M. Schart, L. Bührend, E. Meidinger, J.-J. Kang, B.-J. Niebuur, S. Ariaee, D. S. Molodenskiy, D. Posselt, H. Amenitsch, C. Tsitsilianis, and C. M. Papadakis, Adv. Funct. Mater. 31, 2102905 (2021).

Primary author: Ms YAZDANSHENAS, Bahar (Fachgebiet Physik weicher Materie, Physik-Department, Technische Universität München)

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Presenter: Ms YAZDANSHENAS, Bahar (Fachgebiet Physik weicher Materie, Physik-Department, Technische Universität München)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Investigation of the microstructural evolution during hot deformation and cooling in VDM® Alloy 780 by in-situ high-energy X-ray diffraction

Friday, December 9, 2022 4:35 PM (25 minutes)

Ni-based superalloys are essential for applications in demanding environments, such as jet engines or the heavily stressed rotating discs in the hot sections of modern gas turbines. Such environments typically challenge the material with a combination of high temperatures, high tensile loads, and oxidizing atmospheres. In this study, the polycrystalline Ni-based superalloy VDM 780® Alloy 780 was investigated consisting of γ-matrix, γ'-hardening phase, δ and η high-temperature phases. High-energy X-ray diffraction experiments were performed in-situ during hot compression with synchrotron radiation to mimic the forging process in this study. In the first part of the experiments, i.e. the hot forming, the formation, and development of the crystallographic texture were investigated. During plastic deformation, subgrain formation, rotation of the grains into preferred orientations, and dynamic recrystallization were observed. In the second part, directly after the hot forming at 1000 ℃, the microstructural evolution at cooling rates of 10 ℃/min, 100 ℃/min, and 1000 ℃/min were investigated in situ. Post dynamic recrystallization, grain growth, and precipitation of γ' can be observed, and their magnitude is strongly influenced by the cooling rate. Advanced microscopy techniques confirmed the diffraction results and showed that the recrystallized fraction is highest at the slowest cooling rate and vice versa.

Primary author: Dr FRITTON, Massimo (Technische Universität München)

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Presenter: Dr FRITTON, Massimo (Technische Universität München)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **32** Type: **Invited talk (30 min + 5 min discussion)**

Neutron Diffraction in Pulsed Magnetic Fields up to 40 Teslas

Thursday, December 8, 2022 3:00 PM (25 minutes)

The last two decades have seen the demonstration of the feasibility of neutron diffraction in fields as high as 40 T with the development of dedicated pulsed field devices based either on short or long duration pulsed magnets [1, 2]. These breakthroughs have allowed to extend the field limits beyond current superconducting (15 T split, 17 T solenoid) and resistive installations already available at radiation sources and have allowed to reveal novel field induced states. However, diffraction measurements in high magnetic field environment remain challenging, and successful campaigns at neutron sources require adequate topic selection and expert preparation.
Here, I will present an overview of the 40-T pulsed field-cryomagnet developed by the LNCMI-Toulouse, the ILL-Grenoble, and the CEA-Grenoble, illustrated by a selection of results obtained on the triple-axis CRG-CEA spectrometer IN22 at the ILL. This will give me the opportunity to discuss technical challenges and improvements required to pave the way for the routinely investigations of materials bearing small magnetic moments like, e.g., high Tc superconductors or quantum spin systems.

[1] S. Yoshii et al., Phys. Rev. Lett. 103, 077203 (2009).
[2] F. Duc, et al., Rev. Sci. Instrum. 89, 053905 (2018).

Primary author: Dr DUC, Fabienne (Laboratoire National des Champs Magnétiques Intenses - CNRS)

Presenter: Dr DUC, Fabienne (Laboratoire National des Champs Magnétiques Intenses - CNRS)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **33** Type: **Poster**

KOMPASS –the polarized cold neutron triple-axis spectrometer at the FRM II

Friday, December 9, 2022 3:30 PM (1h 30m)

KOMPASS is a polarized cold-neutron three axes spectrometer (TAS) currently undergoing its final construction phase at the MLZ in Garching. The instrument is designed to exclusively work with polarized neutrons and optimized for zero-field spherical neutron polarization analysis for measuring all elements of the polarization matrix. In contrast to other TASs, KOMPASS is equipped with a unique polarizing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam. The exchangeable straight and parabolic front-end sections of the guide system allow adapting the instrument resolution for any particular experiment and provide superior energy- and Q-resolution values when compared with the existing conventional guide and instrument concepts [1, 2]. In combination with the end position of cold neutron guide, the large doubly focusing HOPG monochromator and analyzer, the V-cavity for analysis of polarization of scattering beam, the KOMPASS TAS will be very well suited to study various types of weak magnetic order and excitations in variety of complex magnetic structures and indeed first successful experiments on chiral magnets or very small crystals could already be performed.
[1] M. Janoschek et al., Nucl. Instr. and Meth. A 613 (2010) 119.
[2] A. C. Komarek et al., Nucl. Instr. and Meth. A 647 (2011) 63.
The construction of KOMPASS is funded by the BMBF through the Verbundforschungsprojekt 05K19PK1.

Primary authors: GRÜNWALD, Alexander (Institute of Physics II, University of Cologne); Dr GORKOV, Dmitry (FRM2); WALDHERR, Georg; STEIN, Jonas (Institute of Physics II, University of Cologne); MÜLLER, Manuel (FRM2); BRADEN, Markus (Universität zu Köln); BÖNI, Peter (Technische Universität München); GIEMSA, Stefan

Presenter: Dr GORKOV, Dmitry (FRM2)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **34** Type: **Talk (20 min + 5 min discussion)**

Combined PGAA and in-beam NAA measurements on mineral

Thursday, December 8, 2022 1:40 PM (25 minutes)

Heavy mineral separates from Hungarian sand samples were measured by instrumental NAA at the Budapest Research Reactor (BRR), but the amounts and weights of them were way too small to also analyze them effectively at the PGAA station of the BNC. Combined PGAA and in-beam NAA experiments were made on the samples at FRM-II to study their possibilities.
First, the mineral separates were irradiated at the PGAA station with an elliptically focused neutron beam (Φth: 4x1010 cm-2s-1) and the emitted decay gammas were measured for 15 minutes in situ. Then, the samples were moved to a low-background counting chamber for longer decay gamma counting. After the short-time and high-flux irradiations for in-beam NAA measurements, long irradiations followed by decay counting were run at the PGAA.
Compared to the INAA results, we detected 12-14 more elements and their precise mass fractions by PGAA and in-beam NAA at FRM-II. The analyses based on the decay spectra acquired at PGAA yield only few elements (e.g. Eu, Dy, and Br), which can be better detected in the low-background chamber. The decay measurement at the irradiation position seems to be reasonable for short-lived nuclides only.
PGAA and INAA complement each other; their combination offers a panoramic analysis for a much broader circle of elements. Their unique opportunities must be further investigated at the two European PGAA-INAA facilities (MLZ and BNC) to enhance the quality assurance and control.

Primary authors: Dr GMÉLING, Katalin (Centre for Energy Research); Dr RÉVAY, Zsolt (Technische Universität München, FRM-II)

Co-authors: Dr STIEGHORST, Christian (Technische Universität München, FRM-II); Dr SZENTMIKLÓSI, László (Centre for Energy Research)

Presenter: Dr GMÉLING, Katalin (Centre for Energy Research)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **35** Type: **Poster**

Residual stresses in Cu matrix composite surface deposits manufactured via laser melt injection

Friday, December 9, 2022 3:30 PM (1h 30m)

Metal matrix composite (MMC) coatings can improve surface wear resistance significantly. However, both macro and micro residual stresses exist in the MMC coatings, causing detrimental effects such as reducing service life. Based on neutron diffraction, we determined the residual stresses in the spherical fused tungsten carbide (sFTC) reinforced Cu matrix composite surface deposits after laser melt injection. A thermo-mechanical coupled finite element model was also developed to predict the residual stresses. We found that the residual stresses are low in the sFTC/Cu composite deposit produced with 400 ℃ preheating temperature, with a maximum tensile residual stress of about 100 MPa in the Cu matrix on the top surface. In contrast, the residual stresses in the sFTC/bronze (CuAl10Ni5Fe4) composite deposit are very high. The maximum tensile residual stress in the Cu matrix of the sFTC/bronze composite deposit reaches about 650 MPa on the top surface. The present investigations can help to control the residual stresses in the Cu matrix composite surface deposits and thus increase the service life of wear-resistant coatings in the future.

Primary author: ZHANG, Xingxing

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Presenter: ZHANG, Xingxing

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **36** Type: **Poster**

Experimental proposal using neutron scattering for structural study of hydrated silks

Friday, December 9, 2022 3:30 PM (1h 30m)

Natural protein fibers, silks, are expected as sustainable structural materials because of their excellent mechanical properties, especially the high-toughness nature with a good balance of strength and extensibility. However, the structural origin of the high-toughness of silks has not been well understood. So far, we have studied the hierarchical structure of many kinds of silks on the basis of small-angle and wide-angle X-ray scatterings (SWAXS) and revealed their hierarchical fibrillar structures. Each nanofibril has a periodic repeating structure of crystalline and amorphous phases associated with the specific amino acid sequence. In-situ synchrotron SWAXS measurements during the fiber stretching deformation revealed an essential role of amorphous phase in generating high-toughness nature (Yoshioka T. et al., Nat. Commun. 2019, 10, 1469). On the other hand, silks are known to show high moisture absorption (or hydration) and thus the study on structural deformation process under hydrated state is also very important. However, the SAXS study of hydrated silks gives only poor information because of poor electron density contrast between crystalline and hydrated amorphous phases especially in the stretched state. Here, we want to propose and discuss some experimental designs using neutron scattering for clarifying the structural deformation process of silks under hydrated state as well as some other uncleared structural subjects of silks.

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Session Classification: Poster Session

Track Classification: Material Science

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

Micrometer positron beam at the Scanning Positron Microscope

Friday, December 9, 2022 3:30 PM (1h 30m)

Positron annihilation lifetime spectroscopy is a powerful tool in a wide range of 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 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 needed to reach a lateral resolution in the micro-meter range. An essential component of the interface is the 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 the SPM, which has become a complete makeover during the reactor shutdown. In addition, the latest developments of the positron elevator and the newly developed frequency stabilization system are reported. To ensure proper operation of SPM at NEPOMUC, stable amplitude, stable frequency and stable phase of the RF-signal are crucial.

Primary author: MITTENEDER, Johannes

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Presenter: MITTENEDER, Johannes

Session Classification: Poster Session

Track Classification: Positrons

Contribution ID: **38** Type: **Invited talk (30 min + 5 min discussion)**

Positron Annihilation Lifetime Spectroscopy (PALS) studies of thin film Solar Energy Materials using PLEPS

Thursday, December 8, 2022 1:05 PM (35 minutes)

Orthorhombic Barium di-silicide (BaSi2) is an emerging sun light conversion material for thin film solar cells, owing to its suitable bandgap, high light absorption coefficient, and long minority-carrier lifetime. Moreover, Ba and Si are very abundant and environmentally benign materials. The nature of defects in BaSi2 thin films grown by Molecular Beam Epitaxy (MBE), Thermal Evaporation (TE), and RF-sputtering is examined by PALS. Comparison with ab-initio calculations indicates that Si mono-vacancies are present inside grains of MBE grown BaSi2 films, that have been successfully applied in p-type BaSi2/n-type c-Si heterojunction solar cells. A grain boundary trapping model is employed to unravel the annihilation channels inside the grains and at the grain boundaries, in combination with POSWIN analysis. PALS demonstrates that larger open volume defects, Ba mono-vacancies or di-vacancies, are present in TE-deposited BaSi2 films. BaSi2 films deposited by RF-sputtering will also be discussed. Face-to-Face-Annealing (FTFA) annealing of these films produces orthorhombic BaSi2 and prevents to a large degree near-surface oxidation.
A second class of rapidly emerging thin film solar cells is based on hybrid organic-inorganic lead halide perovskites, that show great prospects for application in perovskite/c-Si tandem cells. PALS studies of formamidynium-based lead halide (FAPI) perovskite absorber layers will be presented and compared to other perovskite studies.

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Presenter: Dr EIJT, Stephan (Delft University of Technology)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **39** Type: **Talk (20 min + 5 min discussion)**

Planned Experiments with the Pulsed Positron Beams PLEPS and SPM

Thursday, December 8, 2022 1:40 PM (25 minutes)

The pulsed positron beams PLEPS and SPM are user facilities at the intense positron source NEPOMUC for defect depth-profiling by means of positron lifetime measurements.

PLEPS uses a monochromatic pulsed positron beam of variable implantation energy and 1 mm diameter. It enables a quantitative and non-destructive characterization of open volume defects, e.g. vacancies, grain boundaries, precipitates or vacancies clusters close to surfaces and in thin films (< 30 nm) and layered structures. With PLEPS in situ manipulation of the sample is possible: The sample temperature can be varied between 80 K and 600 K. With a new broad band illumination system optically active defects can be detected and identified by manipulating their charged states. Positron drift experiments to explore interfaces and internal surfaces can be performed by applying bias voltages to the samples. Typical applications comprise the defect identification in semiconductors and insulators, the investigation of irradiation induced defects in materials for fusion and fission, as well as the characterization of nano-voids in glasses, polymers and polymeric membrane layers.

The positron microscope SPM enables in addition to depth profiling to scan and focus the pulsed beam onto a sample with spot sizes in the range of 1 µm. The lateral resolution allows to investigate 3-dimensional defect distributions. The SPM is in the final stage of commissioning and will be operated in the near future.

Primary author: DICKMANN, Marcel

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Presenter: DICKMANN, Marcel

Session Classification: Positrons

Track Classification: Positrons

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

RESEDA - Resonant spin-echo for diverse application

Friday, December 9, 2022 3:30 PM (1h 30m)

The neutron spin echo spectrometer RESEDA (Resonance Spin Echo for Diverse Applications) is dedicated to the exploration of slow dynamics and fluctuations in hard and soft condensed matter systems. RESEDA is located at the end position of NL5-S in the Neutron Guide Hall West. Following a major revision and upgrade, RESEDA now permits longitudinal NRSE (LNRSE) spectroscopy as well as longitudinal MIEZE (Modulation of Intensity with zero effort) operation with sub-μeV energy resolution and an unprecedented dynamic range. When operated as a MIEZE spectrometer, data may be recorded readily in depolarizing sample environments, such as very large magnetic fields. Likewise, depolarizing substances, such as ferromagnets or superconductors, strong incoherent scattering materials containing, for instance, hydrogen may be studied.

Primary authors: JOCHUM, Johanna K.; BEDDRICH, Lukas (Heinz Maier-Leibnitz Zentrum (MLZ))

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Presenter: WILD, Peter

Session Classification: Poster Session

Track Classification: Neutron Methods

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

Extending MIEZE spectroscopy towards thermal wavelengths

Friday, December 9, 2022 3:30 PM (1h 30m)

We propose a Modulation of intensity with zero effort (MIEZE) set-up for high-resolution neutron spectroscopy at momentum transfers up to 3Å^{-1},energy transfers up to\, 20\,meV, and an energy resolution in the μeV-range using both thermal and cold neutrons. MIEZE has two prominent advantages compared to classical neutron spin-echo. The first one is the possibility to investigate spin-depolarizing samples or samples in strong magnetic fields without loss of signal amplitude and intensity. This allows for the study of spin fluctuations in ferromagnets, and facilitates the study of samples with strong spin-incoherent scattering.
The second advantage is that multi-analyzer setups can be implemented with comparatively small effort. The use of thermal neutrons increases the range of validity of the spin-echo approximation towards shorter spin-echo times. In turn, the thermal MIEZE option for greater ranges (TIGER) closes the gap between classical neutron spin-echo spectroscopy and conventional high-resolution neutron spectroscopy techniques such as triple-axis, time-of-flight, and back-scattering. To illustrate the feasibility of TIGER we present the details of an implementation at the beamline RESEDA at FRM II by means of an additional velocity selector, polarizer and analyzer.

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Presenter: JOCHUM, Johanna K.

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **42** Type: **Talk (20 min + 5 min discussion)**

Dipolar interactions and spin dynamics in the itinerant ferromagnet Ni

Thursday, December 8, 2022 4:15 PM (25 minutes)

The itinerant ferromagnet nickel has a long history of studies investigating its spin wave and critical, paramagnetic scattering over a large range in temperature. Close to T_C = 631 K, the behavior of Ni, as observed with neutron scattering, is well explained by mode coupling and renormalization group theory calculations based on the isotropic Heisenberg model. According to scaling theory, similar properties are expected for prominent ferromagnetic systems such as Fe, EuO and EuS. However, to understand the static and dynamical scaling properties of these systems the introduction of an additional scaling quantity q_D is required. The dipolar wavevector q_D quantifies the anisotropic, long range dipolar coupling of the electrons. In the long wavelength limit and $q < q_D$, the influence of dipolar interactions becomes dominant leading to a deviation of the universal dynamical scaling function and spin wave dispersion as predicted for pure Heisenberg ferromagnets. This scaling was verified for Fe, EuO and EuS by neutron spectroscopy, but to date no evidence has been found in Ni.

We present our investigations of the critical dynamics in Ni using the extreme energy resolution of the MIEZE spectrometer RESEDA. Our results show excellent overall agreement with spin wave and scaling theory, but imply that the q_D is at least 2 times smaller then previously reported, inducing changes in the dynamic properties at the absolute limit of a modern spectrometer's resolution.

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Presenter: BEDDRICH, Lukas (Heinz Maier-Leibnitz Zentrum (MLZ))

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

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

Combined in-situ Raman and neutron spectroscopy at the cold neutron chopper spectrometer TOFTOF

Friday, December 9, 2022 3:30 PM (1h 30m)

The combination of in-situ Raman and neutron spectroscopy is very powerful in order to investigate the molecular dynamics and chemical reactions inside a sampleat the same time. For this purpose we will introduce our new sample environments to combine quasi elastic (QENS) and inelastic (INS) neutron spectroscopy with Raman spectroscopy. To measure Raman and neutrons at the same time it is necessary to include a Raman spectrometer into the available space at the neutron spectrometer TOFTOF. For the Raman spectrometer, we use a commercial available transportable setup, which we can easily install at TOFTOF. The sample can be placed in different sample holders. Each sample holder offers unique possibilities to expose the sample to various environments and stimuli. In this way, we are able to perform measurements within a temperature range of 0 - 100℃. At the same time, it is possible to excite the sample by optical light or to change the humidity. We will present first results of the Raman spectrometer installed at TOFTOF and discuss scientific applications of this combination of techniques.

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Presenter: WOLF, Marcell (TUM)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

In situ precipitation of CoRe alloys studied via neutron and synchrotron methods

Friday, December 9, 2022 3:30 PM (1h 30m)

In the field of gas turbines, the goal of high-temperature alloy development is to reach higher service temperatures including lowering the consumption of the fuel, making the energy production/transformation more efficient and more economical. Our efforts in this area was to develop a new cobalt rhenium (CoRe) base superalloy. Various techniques such as neutron, electron and X-ray based methods are applied to study the microstructure under various environments of temperature and external forces.
High-temperature CoRe based alloys were developed for applications up to 1200℃. The strengthening is performed with a dispersion of nanosized tantalum carbide (TaC) precipitates. The cooling rate from the supersolution stage has strong influence on the size and volume fraction of the precipitates. Various cooling rates and the influence of Cr addition in the alloy were studied mainly with wide-angle and small-angle neutron scattering to monitor in situ the TaC precipitate behaviour under such external parameters.
The isochronal cooling processes are described with the Kampmann–Wagner's numerical (KWN) model. The in-situ measurements give the unique possibility to calibrate the model parameters, whereas the ex situ measurements are used to assess the model predictions.

Reference:
1.) L. Karge, R. Gilles, D. Mukherji, D. Honecker, P. Beran, P. Strunz, M. Hofmann, N. Schell, J. Rösler, S. Busch, Advanced Engineering Materials (2021), 2100129.

Primary author: GILLES, Ralph

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Presenter: GILLES, Ralph

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **45** Type: **Talk (20 min + 5 min discussion)**

On symmetry relationships of binary metallic graphite intercalation compounds structure family - understanding staging transition mechanism and a helpful tool for neutron diffraction studies

Thursday, December 8, 2022 5:10 PM (25 minutes)

Graphitic materials have historically a huge technological importance due to their manifold interesting properties, which mostly arise from the anisotropic bonding arrangement. The weak interlayer bonding opens the capability for intercalation reactions and formation of graphite intercalation compounds (GICs), of special interest are the binary metallic GICs, which are well-known in two families of compounds, MC6 and MC8. Additionally, the high reversibility of the intercalation reaction made graphite-based anode materials commonly used in lithium-ion batteries (LIBs). We reviewed all existing binary stage-1 GIC structure reports from the ICSD-database and other sources and explore the symmetry relationships of these structures by applying group-subgroup considerations. This review gives new insights on the structure building forces in GICs and adds a new view on the phase transition mechanisms between intermediate stages for GICs depicted in the family tree. This can improve detailed neutron diffraction analysis as it helps to identify the structural origins of small deviations in diffraction patterns easily, based on the symmetry relationships of the crystal structures and help to control aging and cell performance characteristics in the Li-GIC system in LIBs, since despite very detailed neutron diffraction studies, still many open questions remain in the complex Li-GIC system.

Primary author: SEIDLMAYER, Stefan

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Presenter: SEIDLMAYER, Stefan

Session Classification: Structure Research

Track Classification: Structure Research

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

High accuracy positioning with an industrial robot system for neutron residual stress and textre analyses at STRESS-SPEC

Friday, December 9, 2022 3:30 PM (1h 30m)

STRESS-SPEC was one of the first neutron diffractometers at which industrial robots for sample handling and positioning were used. However, industrial robots are still limited in their use due to insufficient absolute positioning accuracies of up to ± 0.5 mm in some cases. Usually, an absolute positioning accuracy of 10% of the smallest gauge volume size –which in case of modern neutron diffractometers is in the order of 1×1×1 mm3 –is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. The original robot setup at the neutron diffractometer STRESS-SPEC has therefore been upgraded to a high accuracy positioning/metrology system. We will give a short introduction on the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 µm or better during measurement of the full strain tensor, the sample position is tracked by an optical metrology system and actively corrected, which we will show in detail.
Two new designed radial collimators create more space in the sample environment and enhance the residual stress analysis capabilities for large complex parts. In addition, a newly designed laser furnace can be mounted at the robot flange to conduct, for example, texture measurements at elevated temperatures of up to 1300 ℃. A brief overview of the STRESS-SPEC instrument and its capabilities using the new robot setup will be given.

Primary authors: Mr LANDESBERGER, Martin (TUM); WANG, Lijiu; HOFMANN, Michael; KRUEGER, Jens; Mr KEDILIOGLU, Oguz (FAPS); GAN, Weimin (Helmholtz-Zentrum Hereon)

Presenter: WANG, Lijiu

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **47** Type: **Talk (20 min + 5 min discussion)**

Non-collinear long-range coupling in modulated manganites.

Thursday, December 8, 2022 5:10 PM (25 minutes)

Non-volatile and tunable non-collinear magnetic structures in thin films are gaining increasing importance for several spintronics applications, such as triplet spin-valves, or devices based on the topological Hall effect. Non-volatile non-collinearity can be tailored in heterostructures that exhibit exchange bias or long-range couplings, as the RKKY. We report on the experimental observation of a novel, complex non-collinear structure based on the imprinting of canted antiferromagnetism of the spacer to the neighboring ferromagnetic layers [1]. We studied superlattices composed of optimally doped (x=0.4) ferromagnetic $La_{1-x}Sr_xMnO_3$ of fixed thickness and overdoped (x=0.8) spacer of variable thickness. High hole diffusion over several unit cells creates depth-modulated manganite homojunctions, with an overall complex magnetism that differs from that of its singular components. In particular, at intermediate spacer thickness, we obtained a non-collinear synthetic antiferromagnet, which we investigated by means of polarized neutron reflectometry and diffraction. The novel long-range non-collinear structure is a non-volatile phase which is easily tuned with application of small magnetic fields (H<100 mT).

[1]. Guasco, L., Khaydukov, Y., Kim, G., et al., Emergent Magnetic Fan Structures in Manganite Homojunction Arrays. Adv. Mater. 2022, 34, 2202971. https://doi.org/10.1002/adma.202202971

Primary author: GUASCO, Laura

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Presenter: GUASCO, Laura

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

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

Concept study of an indirect spectrometer of mushroom type at the reactor source FRM II

Friday, December 9, 2022 3:30 PM (1h 30m)

Mushroom is a concept of an indirect neutron spectrometer with a secondary spectrometer based on a super flat-cone analyser made of highly oriented pyrolytic graphite with an array of position-sensitive detectors (PSD) below it. This combination of the analyser and PSD gives the complete information of the outgoing wave vectors from each detected point on the PSDs. The idea has been first presented by R. Bewley for a new spectrometer at the spallation source ISIS in the UK. We aim to adapt the Mushroom concept to the reactor source at FRM II, such that a much higher count rate can be reached than at a traditional triple-axis spectrometer (TAS). This is possible thanks to the special analyser in Mushroom covering a solid angle up to 2π steradian. This allows for obtaining an overview of the dispersion relation and/or diffuse scattering with only a few scans. We report on the theoretical calculations of matching the resolution function of the secondary to the primary spectrometer using monochromatized neutrons from one of the neutrons guides of FRM II. Besides this McStas simulations are presented showing predictions on the instrument performance.

Primary author: TANG, Ran (Technical Univertsity Munich)

Co-author: GEORGII, Robert

Presenter: TANG, Ran (Technical Univertsity Munich)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **49** Type: **Poster**

In Situ Investigation of the Domain Morphology and Doping Level of Thermoelectric PEDOT:PSS Thin Films under Different Ambient Conditions

Friday, December 9, 2022 3:30 PM (1h 30m)

Thermoelectric (TE) generators are considered a promising technique for heat waste recovery as they enable a direct conversion of a temperature gradient into electrical power. Especially polymer based organic thermoelectric materials, like the blend poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS), are very advantageous, as these materials allow a large scale, low-cost solution based processability of low or non-toxic, lightweight and flexible TE devices, with a wide range of applications. For improving the TE performance of PEDOT:PSS thin films, the post-treatment with ionic liquids (ILs) has turned out to be very promising, as two important TE parameters, Seebeck coefficient (S) and electric conductivity (σ), can be increased simultaneously. However, to make these IL post-treated PEDOT:PSS thin films usable in future commercial TE devices it is indispensable to also investigate the performance of these materials for their long-term stability under different ambient conditions, like elevated temperature or increased humidity. Therefore, in this work we examine the effect of different external influences on the thermoelectric properties, and correlate it with changes in the inner film morphology and oxidation level, by performing in situ GISAXS and in situ UV-vis measurements

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Presenter: OECHSLE, Anna Lena (TU München, Physik-Department)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Tunable mesoporous and optoelectronics properties of zinc titanate films using sol-gel technique

Friday, December 9, 2022 3:30 PM (1h 30m)

Mesoporous films consisting of zinc titanate have high potential applications in photocatalysis, solar cells, and sensors due to tailoring their semiconductive properties. In the present work, we investigate the morphologies of mesoporous zinc titanate films obtained by changing the ratio of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer poly(styrene)-b-poly(ethyleneoxide) PS-b-PEO self-assembles into core-shell micelles in a mixture of N,N-dimethylformamid/hydrogen chloride playing the role as structure directing template. The inorganic precursors, zinc acetate dehydrate and titanium tetraisopropoxide, are loaded in the micellar shell due to hydrogen bonds between PEO and precursors. We use slot-die and spin-coating methods to prepare hybrid films, and investigate the influence of the different deposition methods on the film morphologies. Moreover, we investigate how mesoporous structures and crystal phases depend on calcination temperature, concentration and the ratio of two precursors. The morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering (GISAXS) and scanning electronic microscopy (SEM). The film thickness, crystal phase, chemical composition and optical properties are characterized using X-ray reflectivity, X-ray diffraction, Fourier transform infrared spectroscopy, and ultraviolet-visible spectroscopy, respectively.

Primary author: LI, Yanan

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Presenter: LI, Yanan

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **51** Type: **Poster**

Quenching and Deformation Dilatometer for In-Situ Materials' Characterization by Neutron Scattering

Friday, December 9, 2022 4:35 PM (25 minutes)

A Quenching and Deformation Dilatometer (TA instruments DIL 805A/D/T) operates at the MLZ for performing in-situ neutron diffraction (phase, texture, stress/strain) at STRESS-SPEC and small-angle neutron scattering (nanostructure) at SANS-1. Imaging applications are under preparation at ANTARES. With this setup, the evolution of the sample length during heating or quenching can be accurately monitored while scattering data are being acquired. Thanks to induction heating and gas cooling very high rates are accessible. Forces up to 20 and 8 kN can be applied in compression and tension, respectively. Besides, special sample holders for powders will soon extend the range of applications.

The combination of the neutron scattering and dilatometry measurements yields a unique view on the microstructural evolution under thermomechanical treatment. In this work, we will present some results of different materials, i.e. high entropy alloy (HEA), light weight TiAl alloy and Cu-$Ce_{0.8}Gd_{0.2}O_{2-\delta}$ (CGO) composites. Dilatometry and in-situ diffraction allows an accurate investigation of phase transformations in AlCrFeNiTi HEA. TiAl alloy study will be focused on the bulk texture evolution induced by hot compression performed with the dilatometer. Finally, Cu-CGO cermets were studied as a bulk at the same time as we obtain in-situ high temperature microstructural information on both Cu and CGO phases (diffraction measurements performed at the synchrotron Desy).

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Presenter: SOLIS, Cecilia

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **52** Type: **Poster**

Study of the hardening phase precipitation by in-situ high temperature neutron scattering in the new VDM® Alloy 780

Friday, December 9, 2022 4:35 PM (25 minutes)

In order to improve the microstructure and mechanical properties of the 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, fraction 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 microscopy (SEM) provided further details on microstructural and chemical composition.

The precipitation of γ'phase at 720 ℃, i.e. its size and volume fraction 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 result in different precipitates nucleation and growth kinetics. A final heat treatment at 620 ℃ does not lead to a similar precipitation or growth process.

Primary authors: SOLIS, Cecilia; KIRCHMAYER, Andreas (Friedrich-Alexander-Universität Erlangen-Nürnberg); KÜMMEL, Frank (TUM/FRMII); Dr DA SILVA, Ivan (ISIS); MUEHLBAUER, Sebastian; BERAN, Premysl (Nuclear Physics Institute CAS); Dr HAFEZ, Masood (VDM Metals); Dr GEHRMANN, Bodo (VDM Metals); NEUMEIER, Steffen (Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg); GILLES, Ralph

Presenter: SOLIS, Cecilia

Session Classification: Poster Session

Track Classification: Material Science

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

Influence of Solvent and Lithium Salt on the Structure and Performance of NCM111 Cathode for All-Solid-State Lithium Batteries

Friday, December 9, 2022 3:30 PM (1h 30m)

Lithium ion batteries (LIBs) with a wide range of applications have emerged as the most promising candidate for electrochemical energy storage due to its higher specific energies, volumetric energy densities and power densities. However, lithium dendrite will grow and the Coulombic efficiency (CE) will decrease with Li plating and stripping. During past decades, more and more state-of-art materials has been developed to alleviate the abovementioned problems. Nevertheless, fundamental research on the component composition and the effect of additive and solvent on LIBs is still lacking. It is of great value to get a deeper understanding and therefore optimize the fabrication process for future studies on the electrode/electrolyte interface of LIBs. In this project, we select LiNi0.33Mn0.33Co0.33O2 as cathode material to find out the effect of different solvents and extra lithium salt (LiTFSI) on the performance of LIBs. The Li/cathode cells are assembled to observe the battery performance and grazing incidence wide-angle X-ray scattering (GIWAXS) is used to detect structure change within the cathode before and after cycling.

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Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **54** Type: **Poster**

The Effects of Residual Lead Iodide on the Stability of Perovskite Solar Cells

Friday, December 9, 2022 3:30 PM (1h 30m)

Over the past few years, hybrid perovskite materials have attracted tremendous interest due to its excellent photovoltaic properties in perovskite solar cells (PSCs) resulting in record power conversion efficiencies. The residual lead iodide is easy to form during the fabrication of perovskite layers, especially in case of the two-step deposition method. In addition, residual lead iodide has been universally used in the state-of-the-art devices to boost the device performance. However, the effects of residual lead iodide on the stability of PSCs has not been fully understood and, therefore, needs to be deeply investigated for further improvement of device performance. Herein, it is shown that residual lead iodide exhibits insufficient stability under continuous light radiation and heating. The photodecomposition products of lead iodide pose a threat to the efficiency and stability of devices. Thus, unstable lead iodide under light radiation and heating is one of the main reasons for the degradation of perovskite device. Therefore, carefully controlling or eliminating the residual lead iodide in perovskite film is one of the critical methods to improve the long-term stability of PSCs.

Primary authors: JIANG, Xiongzhuo (TU München, Physik-Department, LS Funktionelle Materialien); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

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Session Classification: Poster Session

Track Classification: Material Science

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

Morphology control of titania films at low temperature

Friday, December 9, 2022 3:30 PM (1h 30m)

A low-temperature routine to realize inorganic hole-blocking layers (HBLs) is important for the commercialization of perovskite solar cells. Fabricating HBLs at low temperature is energy-saving and compatible with flexible substrates. In this work, titania thin films are synthesized at low temperature with the sol-gel method templated by a diblock copolymer. Tailoring titania film morphology in the low-temperature process is achieved by managing phase separation of the polymer template. The ratio of polymer, precursor, solvent, and catalyst for the sol-gel solution is varied to tune the thin film morphologies. The surface morphologies of films are probed via scanning electron microscopy and GISAXS. The optical properties are examined with ultraviolet-visible spectroscopy and photoluminescence spectra.

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Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **56** Type: **Talk (20 min + 5 min discussion)**

Fitting Molecular Dynamics water model parameters to neutron scattering experiments

Thursday, December 8, 2022 5:10 PM (25 minutes)

Molecular dynamics (MD) simulations are a valuable tool to investigate structure and dynamics of samples on the same time- and lengthscales as probed by neutron scattering experiments. Force fields for water and bigger molecules have been established, but can they reproduce neutron scattering experiments?

Different parameter fits for MD water models were made and compared to neutron scattering experiments of water.
For the MD simulation the program LAMMPS was used, subsequently SASSENA to calculate the neutron scattering curves –wide-angle diffraction for structure determination and the incoherent intermediate scattering function to probe the dynamic behaviour of the sample, respectively.

The calculated curves show a satisfactory qualitative agreement with neutron scattering data from the literature but also great potential for improvement of the parameters used in the tested force fields. The ultimate goal is to transfer the findings presented here on the example of water to the investigation of hydrogen storage materials.

Primary author: REICH, Veronika

Co-authors: Prof. MÜLLER, Martin (Helmholtz-Zentrum hereon GmbH); Dr BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany)

Presenter: REICH, Veronika

Session Classification: Soft Matter

Track Classification: Soft Matter

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

Stacking Kinetics of PbS QDs Orientated by Perovskite Matrix during Printing

Friday, December 9, 2022 3:30 PM (1h 30m)

PbS colloidal quantum dots (CQDs) have generated great interests in various optoelectronic devices including solar cells, photodetectors and infrared light-emitting diodes (LEDs), due to their size-tunable bandgap, low-temperature and solution processability. To date, defects and charge carrier transport in CQD solids and surface passivation of one single QD remain major challenges for the performance of QD based devices. In our work, we select perovskite constitutes as the ligand precursors to conduct solution ligand exchange for as-synthesized PbS QDs and the final QD powder is dissolved with n-butylamine to obtain QD ink for slot-die printing. In this work, we focus on how QDs capped with different ligands dynamically stack in the phase transition from QDs ink to a film during slot-die printing by grazing-incidence small-angle X-ray scattering (GISAXS). In addition, the post- treatment annealing and heated substrate during the film deposition are investigated to observe the inner structure of QDs film in real time. Grazing-incidence wide-angle X-ray scattering (GIWAXS) and GISAXS are simultaneously used to investigate how the perovskite ligands form into crystals and how the crystalline orientation of perovskite matrix dynamically aligns and influences the QDs stacking behavior in the final film formation.

Primary authors: ZHONG, Huaying; Prof. MÜLLER-BUSCHBAUM, Peter (Technische Universität München (TUM)); Dr CHEN, Wei (Shenzhen Technology University (STU))

Presenter: ZHONG, Huaying

Session Classification: Poster Session

Track Classification: Material Science

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

In-situ investigation during gold HiPIMS deposition onto polymers

Friday, December 9, 2022 3:30 PM (1h 30m)

Gold deposition *via* high power impulse magnetron sputtering (HiPIMS) allows to coat thin metal layers on heat sensitive materials such as polymers allowing for increased adhesion and density. HiPIMS allows deposition at a lower total deposited thermal energy in comparison to conventional magnetron sputtering, but this energy is delivered in a very short pulse exhibiting very high power and ionization. The consequences for the nucleation and growth processes during HiPIMS deposition are not sufficiently known. Therefore, we investigate the morphology evolution of thin gold layers on four polymer templates, namely polystyrene (PS), polystyrene sulfonicacid (PSS) and poly-4-vinylpyridin (P4VP). These polymers show different functional moieties and thus are expected to influence the growth of the gold layer. First results of the in situ investigations combining grazing-incidence small angle X-ray scattering (GISAXS), grazing incidence wide angle X ray scattering (GIWAXS) will be presented.

Primary author: Mr BULUT, Yusuf (DESY/TUM)

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Presenter: Mr BULUT, Yusuf (DESY/TUM)

Session Classification: Poster Session

Track Classification: Material Science

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

Interaction of colloids with cellulose nanofibrils in aqueous solution

Friday, December 9, 2022 3:30 PM (1h 30m)

Our goal is to fabricate colloidal photonic layers exploiting structural colors in cellulosic materials. The colloidal distribution is a result of the self-assembly of colloidal particles during the drying process after spraying deposition. Therefore, the aim of our experiments is to follow the colloidal layer development during spray coating of colloidal inks used for lay-er formation on nanoporous templates. Cellulose nanofibrils (CNFs) are a wood-based mate-rial with a high aspect ratio (length ~500 nm and small diameter ~5 nm) and a tunable negative surface charge. The aqueous colloidal ink consists of polymer colloids with a completely deuterated and completely protonated and either hydrophobic PMMA core and a cationic hydrophilic PDMAEMA shell. In order to spray these colloids, they were diluted to a final concentration of 0.1 wt in water. The self-assembly of the colloids on CNF films in the wet layer after spray deposition is governed by the colloid-CNF-water interaction. To explore this interaction of the colloids with CNF in the dispersion state typically used for spray coating conditions, we performed small angle neutron scattering (SANS) experiments at D22 of the Institute Laue Langevin (ILL) in Grenoble in cooperation with the Heinz Maier-Leibnitz Zentrum (MLZ). In the fully protonated colloidal suspension, the shape of the colloid nanoparticles can be modeled by a poly disperse core-shell sphere.

Primary authors: Mr HARDER, Constantin (DESY/TUM); Mr ALEXAKIS, Alexandros (KTH); VAGIAS, Apostolos (FRM2 / TUM)

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Presenter: Mr HARDER, Constantin (DESY/TUM)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **60** Type: **Talk (20 min + 5 min discussion)**

Quantum cascade laser-based infrared spectrometer combined with small angle neutron scattering for life science applications.

Thursday, December 8, 2022 5:35 PM (25 minutes)

Using the amide I band, infrared (IR-) spectroscopy can give information on the fold of the protein and also allows to follow aggregation phenomena. Small angle neutron scattering also reports on the global structure of proteins in solution and can give information on the shape of growing aggregates or folded proteins in solution.
We would like to explore the capabilities of infrared spectroscopy based on quantum cascade lasers (QCLs) in combination with small angle neutron scattering (SANS). The advantages of QCLs are superior Gaussian beam characteristics and a higher spectral density as compared to the glow bar infrared light sources of the Fourier-transform infrared spectrometer (FTIR). Their disadvantage is the more complicated pulsed mode of operation and the limited spectral width they can cover.
As a first scientific sample, the effect of a pH drop on protein aggregation and amyloid like structure formation in insulin is investigated. Insulin was dissolved in a phosphate buffer, where the pH was adjusted to 2. At room temperature, the sample was pumped through varying combinations of flow through cells of the FTIR spectrometer, the QCL, the UV-Visible spectrophotometer and the static light scattering device. Thereby we could follow the amyloid like structure formation on the very same sample using many different techniques in parallel. In November we have a scheduled beamtime at SANS-1 at PSI to finally add SANS as one of those techniques.

Primary author: Dr DADFAR, Seyed Mohammad Mahdi

Co-authors: Dr STADLER, Andreas; Dr RADULESCU, Aurel; Prof. FITTER, Jörg; Dr SCHRADER, Tobias

Presenter: Dr DADFAR, Seyed Mohammad Mahdi

Session Classification: Soft Matter

Track Classification: Soft Matter

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

The Electron Microscopy Facility at the MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

In order to provide our users the possibility to complete their neutron scattering data with real space images we will present the Electron Microscopy possibilities at MLZ consisting of a Cryogenic transmission electron microscope Cryo-TEM (JCNS) and an Environmental Scanning Electron Microscope ESEM (JCNS & Hereon).

TEM yield real space images of soft matter systems, particularly in cryogenic environment, in terms of size measurements and distribution of particles, shape, self-assembly systems and aggregates; virtually it may complete and enhance any SANS, reflectometry and macromolecular crystallography on soft matter investigation.
Moreover, the MLZ is, since recently, also equipped with a Thermo Fischer Quattro S Environmental Scanning Electron Microscope (ESEM) operated in conjunction/cooperation by JCNS and Hereon.
Beyond conventional SEM imaging on Material Science samples, the ESEM offers the possibility to work under relatively high pressure and in the presence of humidity and this, without having to subject the sample to any preliminary coating. This will allow investigations of soft matter system with water content. Additionally the ESEM is eqipped with an EDX detector for elemental analysis.
The instruments as well as the extended suite of preparation equipment will be described.

Primary authors: KRIELE, Armin (Helmholtz Zentrum Hereon); APPAVOU, Marie-Sousai (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

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Session Classification: Poster Session

Track Classification: Material Science

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

Exploring the kinetics of Pseudo-bilayer architecture formed during sequential deposition via slot die coating

Friday, December 9, 2022 3:30 PM (1h 30m)

Recently, organic solar cells have received increasing attention due to superior flexibility and being light weight. Among the structures of the active layer, planar and bulk heterojunction structures are commonly adopted, which have their individual intrinsic shortcomings. The new developed pseudo-bilayer structure can perfectly combine their strengths and circumvent their drawbacks. Unfortunately, most pseudo-bilayer films are still prepared by spin coating and there are only few researches about pseudo-bilayer films installed by slot die coating, which is a frequently used roll-to-roll manufacturing technique. Besides these researches mainly focus on selecting suitable solvents, changing donors or acceptors, adding third components and tailoring the vertical morphology. The kinetics of forming the pseudo-bilayer architecture with slot-die coating are still unknown. In the present study, PBDB-T-2F (or PM6) and BTP-4F (or Y6) are selected as donor and acceptor, which will be dissolved in CB and CF, respectively. PBDB-T-2F is firstly slot-die coated on the substrate and then BTP-4F is identically coated on the top of PBDB-T-2F. During the deposition, in situ GIWAXS, in situ GISAXS, and in situ UV-vis absorption spectroscopy experiments are carried on to study the formation of the pseudo-bilayer.

Primary authors: ZHANG, Jinsheng (TU München, Physik-Department, LS Funktionelle Materialien); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: ZHANG, Jinsheng (TU München, Physik-Department, LS Funktionelle Materialien)

Session Classification: Poster Session

Track Classification: Material Science

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

Template-Induced Growth of Sputter-Deposited Gold Nanoparticles on Ordered Porous TiO2 Thin Films for Surface-Enhanced Raman Scattering Sensors

Friday, December 9, 2022 3:30 PM (1h 30m)

Ordered porous gold/titanium dioxide (Au/TiO2) hybrid nanostructured films are specifically interesting in large-scale applications using localized surface plasmon resonances (LSPRs) and surface-enhanced Raman scattering (SERS). In this work, we investigate the optical response of sputter-deposited Au/TiO2 nanohybrid thin films with a focus on the plasmonic response and application as molecular sensors. To elucidate the origin of this behavior, we apply in situ grazing-incidence small-angle X-ray scattering (GISAXS) to investigate the growth kinetics of Au on a TiO2 template during sputter deposition. Based on time-resolved GISAXS, the growth characteristics of sputter-deposited Au on TiO2 template with a final effective Au layer thickness around the percolation threshold are described with the well-known four-stage model of nucleation and cluster formation, diffusion-mediated growth, adsorption-mediated growth and grain growth. The Raman intensity of deposited molecules, probed with rhodamine 6G (R6G), depends on the deposited gold thickness. It shows its maximum at the effective Au thickness (δAu) of 3.4 nm. The maximum in SERS intensity is corroborated by the existence and optimal size of hot spots in the narrow space occurring between the sputter-deposited Au clusters, when staying below the percolation threshold.

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Presenter: LIANG, Suzhe (Technische Universität München)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **64** Type: **Talk (20 min + 5 min discussion)**

Shear flow in spray-deposited cellulose nanofibril dispersions

Thursday, December 8, 2022 4:15 PM (25 minutes)

Fabricating functional material relies on non-equilibrium hydrodynamic flows. Spray deposition using atomization of complex liquids leads to a deposition of droplets on a substrate. The solvent evaporates and induces a complex flow in the dispersion. This leads to a nanostructuring of the nanoscale ingredients of the dispersion. Using cellulose nanofibrils and water as solvent, we have recently established sprayed ultra-smooth nanopaper. Its response to humidity was elucidated via in situ grazing incidence small-angle neutron scattering (GISANS) at KWS-1. Different surface charges of the CNF lead to different nanostructuring owing to the electrostatic repulsion of the CNF. We could find that the cellulose fibrils form a densely packed network with radial distribution to the outer sample regions Yet, the observation of the emerging of the ordering at the liquid-solid interface is hitherto not accessible. Hence, in order to understand the complex flow mechanism in the liquid droplet, we aim in investigating the interfacial shear induced self-assembly mimicking the droplet-substrate interface. Our aim is to understand the formation of the first mono-/bi-layer of CNF suspension on a hard substrate (silicon) as first step of nanopaper formation by applying in situ rheometry.

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

Presenter: ROTH, Stephan (DESY / KTH)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **65** Type: **Poster**

Hybrid Energy Harvester based on the Combination of Triboelectric Nanogenerator and Solar Cell

Friday, December 9, 2022 3:30 PM (1h 30m)

Developing clean energy lies in 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 effect of triboelectrification and electrostatic induction. Compared with other counterparts, owing to the light-weight, low-cost, and easy fabrication, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attentions 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 our 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.

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

Session Classification: Poster Session

Track Classification: Material Science

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

TRISP instrument poster

Friday, December 9, 2022 3:30 PM (1h 30m)

TRISP is currently transferred to the “Neutron Guide Hall East”. A new ballistic neutron guide with elliptic and parabolic sections helps to avoid losses of the neutron flux, although the distance from the reactor increases from 10m to 30m. The ballistic guide also includes a cavity polarizer (length 3.6m) with a good polarization efficiency of ~90% in the wavelength band 1-4 Angström. We will also renew the RF spin flippers, such that the energy resolution is increased by 50%. TRISP will be operational in April 2023.

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

Co-authors: TRALMER, Franz (MPI-FKF); Prof. KEIMER, Bernhard

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

Session Classification: Poster Session

Track Classification: Neutron Methods

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

Influence of thermal effects on combinatorial plasmonic nanostructure for bio-detection

Friday, December 9, 2022 3:30 PM (1h 30m)

In recent decades, Au nanoparticles (NPs) have been utilized in a wide range of sensor applications, such as photodetection, bio-detection, and thermal-detection, because of their unique optical and chemical properties. Among the optical sensors, surface-enhanced Raman spectroscopy (SERS) has attracted extensive attention, being used in the identification of unknown substances in analytical chemistry. In this work, we investigate in situ sputtering Ag on highly ordered Au NPs substrate probe by Grazing incidence small angle X-ray scattering (GISAXS). In addition, we explore the effect of thermal on silver growth kinetic of different sizes of Au substrate. Furthermore, by correlating the growth steps of the composite Au/Ag nanostructures with the SERS performance, we could obtain the plasmonic "hot spot"performance corresponding to the combinatorial nanostructure.

Primary author: GUAN, Tianfu

Co-author: MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: GUAN, Tianfu

Session Classification: Poster Session

Track Classification: Structure Research

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

Operando study of humidity on the performance of perovskite solar cells

Friday, December 9, 2022 4:35 PM (25 minutes)

Perovskite solar cells (PSCs) are among the most promising photovoltaic technologies and reached a certified 25.6% efficiency owing to their tuneable bandgap, high charge carrier mobility, long diffusion length. The long-term operational stability of PSCs, however, has been not investigated in depth. Herein, we probe the structure changes with grazing-incidence small-angle x-ray scattering techniques (GISAXS) under high humidity conditions. 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 a slow decay of VOC, which is correlated to an improved morphology of the active layer and a passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology changes being probed combined with solar cell parameters during the device operation.

Primary author: SUN, Kun

Co-authors: Mr GUO, Renjun (Physics Department, TUM); Mr HEGER, Julian E. (Physics Department, TUM); Mr REUS, Manuel A. (Physics Department, TUM); Mr SPANIER, Lukas V. (Physics Department, TUM); Dr BERNSTROFF, Sigrid (Elettra Sincrotrone); MÜLLER-BUSCHBAUM, Peter (Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien)

Presenter: SUN, Kun

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **69** Type: **Invited talk (30 min + 5 min discussion)**

Neutron scattering under high pressure to 10 GPa and beyond: A brief survey of methods, constraints and science examples

Thursday, December 8, 2022 1:05 PM (35 minutes)

Pressure is next to temperature the key thermodynamic parameter for the exploration of condensed matter. In this talk I will survey the state of the art of high pressure neutron scattering, covering both diffraction and inelastic scattering. I will focus on more recent methods able to reach pressures of 10 GPa and beyond, relevant for research on hard condensed matter. My talk will be largely technical, with an emphasis on the various constraints, and I will give recommendations for potential applications at MLZ.

S. Klotz, Techniques in High Pressure Neutron Scattering, CRC Press –Taylor and Francis, 2013

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Presenter: KLOTZ, Stefan (IMPMC, Sorbonne Université)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **70** Type: **Talk (20 min + 5 min discussion)**

CHARM –A fast, high resolution curved 3He-based Multiwire-Proportional Chamber for the powder diffractometers DMC and ERWiN

Thursday, December 8, 2022 2:05 PM (25 minutes)

As part of the CHARM project, two large area 3He-filled curved Multiwire Proportional Chambers (MWPC) covering 130° horizontal and 14° vertical acceptance have been designed and built by the MLZ detector group in collaboration with the Paul-Scherrer-Institut (PSI). Based on a concept of the Brookhaven National Laboratory, the detector consists of nine individual MWPC segments mounted seamlessly inside a common pressure vessel. Single wire/strip readout using a time-over-threshold based centre-of-gravity (CoG) algorithm is applied aiming at 0.115° angular resolution (FWHM) in both dimensions with 200 kHz global count rate capability per MWPC segment. Filled with 6.5 bar 3He + 1.5 bar CF4 the detector provides 75% detection efficiency for thermal neutrons. At present, the two detectors are under commissioning at the FRM II detector lab and the instrument DMC at PSI, respectively. We will report on the production and tests of the detectors as well as results from the commissioning phase.

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Presenter: ZEITELHACK, Karl

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **71** Type: **Talk (20 min + 5 min discussion)**

In situ GIWAXS investigations of slot-die coated perovskite thin-film materials

Thursday, December 8, 2022 2:05 PM (25 minutes)

Slot-die coating is a versatile and roll-to-roll compatible deposition technique that aims to lower production costs for thin-film-based perovskite solar cells. Our custom-built slot-die coater offers advanced morphology control capabilities and is compatible with in situ GISAXS/GIWAXS (grazing-incidence small/wide-angle X-ray scattering) and photoluminescence measurements [1]. Morphology control of the absorber material is crucial for high performance and reliable product quality. GISAXS/GIWAXS are a powerful combination to investigate the morphology and structure of thin films [2]. Here, we report on the time-resolved phase and quantitative texture evolution during the annealing and printing process of bulk MAPbI3 [3]. Different ordering appears for bulk perovskite depending on the deposition technique (spin-cast vs slot-die coated). We also report on the successful printing of CsFAPbI3 QDs for solar cell applications and report on well-working devices that show the advanced possibilities with pre-deposition crystallized materials.

Primary authors: REUS, Manuel (TUM E13); KOSBAHN, David (TUM E13); REB, Lennart (TUM E13); KRIFA, Ahmed; GUO, Renjun (Physics E13, Technical University in Munich); WEINZIERL, Alexander; LI, Yanan; SCHWARTZKOPF, Matthias (DESY); VAGIAS, Apostolos (FRM2 / TUM); WEINDL, Christian (TUM Physik); XIAO, TIANXIAO (Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München); YIN, Shanshan (Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany); Dr CHUMAKOV, Andrei (DESY); ROTH, Stephan (DESY / KTH); MÜLLER-BUSCHBAUM, Peter (Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany; MLZ, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: REUS, Manuel (TUM E13)

Session Classification: Material Science

Track Classification: Material Science

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

Sustainable biohybrid interfaces: GISANS study on spray deposited whey protein and titania composite films at varying pH

Friday, December 9, 2022 3:30 PM (1h 30m)

Metal oxide interfaces are suitable functional materials for various energy applications. For example, TiO2 can act not only as an anode material in new generation photovoltaic and energy storage technol-ogies, but also in the photocatalytic production of hydrogen. For such applications, a controlled mor-phology on distinct length scales is particularly important to fulfill optimal performance conditions. Furthermore, a high interfacial area and, hence, a high surface-to-volume ratio of nanostructured TiO2 is beneficial for devices. Industrial-relevant deposition methods, such as spray coating, are applicable to fabricate intended morphologies by low-cost solution processing via diblock copolymer-directed sol-gel synthesis. When it comes to an industrial scale, however, limiting factors affecting sustainability are the commonly involved organic solvents. Water-soluble biopolymers can replace synthetic copol-ymers to facilitate sustainable production. The bovine whey protein ß-lactoglobulin (ß-lg) can act as a template in water-based TiO2 synthesis forming aggregates of different structures by denaturing at dif-ferent pH values. In this work, biohybrid films are obtained from solutions with decreasing pH using spray deposition. Bulk and surface-sensitive grazing-incidence small-angle neutron scattering (GISANS) investigations yield an understanding of the influence of pH on the biohybrid film's mor-phologies. Real-space imaging complement the obtained results.

Primary authors: Mr HEGER, Julian (TU München); Ms GEIGER, Christina (TU München); Mr WIDMANN, Tobias (TU München); Dr KREUZER, Lucas P. (TU München); Ms YIN, Shanshan (TU München); Dr KOUTSIOUMPAS, Alexandros (MLZ/JCNS); Prof. MÜLLER-BUSCHBAUM, Peter (TU München/MLZ)

Presenter: Mr HEGER, Julian (TU München)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Imaging from meV to MeV Neutrons at the NECTAR Instrument

Friday, December 9, 2022 3:30 PM (1h 30m)

Located at the SR10 at the FRM II, NECTAR is a versatile instrument and designed for the non-destructive inspection of various objects by means of fission neutron radiography and tomography. Compared to the Z-dependency of X-ray and gamma imaging, fission neutrons have the strong advantage of often providing similar contrast for heavy and light materials. Only few facilities around the world provide access to well collimated fast neutrons, with NECTAR at the FRM II being the only instrument that has a dedicated user program for fast neutron imaging. Aside from fast neutrons, thermal neutron as well as gamma imaging is possible by using different scintillator materials with the same detector system, extending NECTAR's imaging capabilities to different modalities.
Here, we present the most recent upgrades to the NECTAR beam-line, including unparalleled elemental imaging capabilities with examples provided for archaeology, batteries and scintillator materials, as well as recent progress in event-mode imaging with fast neutrons.

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Co-authors: WOLFERTZ, Alexander (TUM FRM2); SOMMER, Lucas; SCHULZ, Michael; KUMAR, Richi

Presenter: LOSKO, Adrian (Technische Universität München, Forschungs-Neutronenquelle MLZ (FRMII))

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **74** Type: **Poster**

Effects of NSAIDs on the Dynamics and Phase Behavior of DODAB Bilayers

Friday, December 9, 2022 3:30 PM (1h 30m)

Dioctadecyldimethylammonium bromide (DODAB), show rich phase behavior [1]. We have studied the effects of Non-steroidal inflammatory drugs (NSAIDs), aspirin and indomethacin, on the phase behavior and the dynamics of DODAB lipid bilayer using quasielastic neutron scattering technique (QENS). Elastic window scan showed that aspirin and indomethacin shifts coagel to fluid phase transition at lower temperatures, compared to pure DODAB. While cooling, aspirin and indomethacin suppresses the intermediate gel phase, found in pure DODAB. QENS data analysis showed that only internal motion exists in coagel phase whereas in fluid phase DODAB involves both lateral and internal motions. In coagel phase, although rotational diffusion coefficient of DODAB is found to be almost twice with both NSAIDs, the dynamically active hydrogen fraction in DODAB becomes twice for aspirin but remains same for indomethacin. In the fluid phase, lateral motion decreases in presence of indomethacin. Whereas, aspirin does not affects lateral motion. DODAB internal motion remains unchanged in presence of indomethacin, whereas, aspirin enhances the internal motion of DODAB. This study reveals that NSAIDs, aspirin and indomethacin affects DODAB lipid bilayer phase and dynamics uniquely.

1. F-G Wu, N-N Wang, Z-W Yu. *Langmuir* **25**, 13394–13401 (2009).
2. P S Dubey, H Srinivasan, V K Sharma, S Mitra, V Garcia Sakai and R Mukhopadhyay, *Scientific Reports* **8**, 1862 (2018).

Primary author: Dr DUBEY, Purushottam (JCNS - 4)

Presenter: Dr DUBEY, Purushottam (JCNS - 4)

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **75** Type: **Talk (20 min + 5 min discussion)**

Multimodal Imaging capabilities at MLZ

Thursday, December 8, 2022 3:25 PM (25 minutes)

The imaging group at MLZ operates the instruments ANTARES and NECTAR. ANTARES provides a cold neutron spectrum and is suitable for high spatial resolution imaging, capable of detecting small compositional changes in millimeter to centimeter sized samples. NECTAR is a fission neutron-imaging instrument, suitable for investigating large samples with sample sizes up to several tens of centimeters.
To complement both techniques, cold and fission neutron imaging, ANTARES is being upgraded with an X-ray source placed perpendicular to the neutron beam to allow for simultaneous X-ray and neutron tomography to complement the cold neutrons. At NECTAR, with the production of fission neutrons, gamma rays are inherently produced as by-products and can be utilized for multimodal imaging by using gamma-sensitive scintillator screens in place of the neutron scintillators, viewed by the same camera. Similarly, thermal neutrons at NECTAR can also be utilized for imaging applications.
With multi-modal imaging capability upgrades at both instruments, we present the current state of these developments, including detailed insight to the setups along with first application examples.

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Presenter: KUMAR, Richi

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **76** Type: **Talk (20 min + 5 min discussion)**

Event Mode Neutron Imaging with ns Temporal and µm Spatial Resolution

Thursday, December 8, 2022 3:00 PM (25 minutes)

Recent developments in event driven camera systems allow the construction of a new type of scintillator-based event mode imaging devices. A neutron imaging device employing this new technology to reach high spatial and temporal resolution is currently under development at the NECTAR instrument at FRMII. The goal is for the detector to have a spatial resolution better than 100 µm and a timing resolution of 10 ns. At the same time, the individual neutron detection approach should improve the signal to noise ratio. With high temporal and spatial resolution, the detector can be used in applications where timing and location are critical, such as high-resolution time of flight imaging and modulation of intensity with zero effort (MIEZE).

The structure of the detector consists of a scintillator screen, an image intensifier and a photosensitive sensor with single photon readout. A lens is used to collect the light from the scintillating screen on the image intensifier. The setup is flexible and allows an easy change of the scintillator screen and the field of view.

A working prototype has already been built and successfully tested. The current development is focused on determining the properties of different scintillating screens and categorize them with respect to their usefulness in achieving the targeted detector parameters. First results from different scintillators will be presented at the MLZ user meeting.

This project is funded by the BMBF under the grant number 05K22WO5.

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Presenter: SCHULZ, Michael

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **77** Type: **Talk (20 min + 5 min discussion)**

Development of a workflow to calculate the X-ray and neutron diffraction pattern from continuum simulations of macroscopic structures

Thursday, December 8, 2022 3:50 PM (25 minutes)

It is a common practice in science to approach a problem simultaneously from the theoretical and experimental side. However, it is important to compare theory and experiment as directly as possible in order to validate that the theory describes reality. This contribution focuses on bridging the gap between simulations and scattering experiments with neutrons and X-rays.
Although scattering experiments are a very powerful tool to understand the structure and dynamics of materials on the nanoscale, the analysis of scattering patterns suffers from underdetermination, i. e. different structures can yield the same scattering pattern. One way to help alleviate this phase problem is to run a molecular dynamics (MD) simulation and calculate scattering patterns from it. However, this approach reaches its limits for large systems due to the myriad amount of computation time required.
This work tries to create a workflow in order to generate scattering patterns of large structures with continuum descriptions, i. e. structures that are continuous instead of a summation of atoms. Our final vision is to separate the scattering pattern of inhomogeneities of a macroscopic sample from its environment.

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Presenter: MAJUMDAR, Arnab (Helmholtz Zentrum hereon)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **78** Type: **Poster**

The cold neutron imaging beam line ANTARES

Friday, December 9, 2022 3:30 PM (1h 30m)

The cold neutron imaging beam line ANTARES at FRM II is a state of the art facility, which combines excellent beam properties with highly flexible experimental conditions. User experiments can be performed with complex sample environment like croystats, furnaces or tensile rigs.
In this poster, we give an overview of the beam line layout and possible options of the beam line. Moreover, we will show examples of selected experiments performed at ANTARES to demonstrate the potential of the beam line.

Primary author: SCHULZ, Michael

Co-authors: SCHILLINGER, Burkhard; NEUWIRTH, Tobias; SEBOLD, Simon (MLZ); TARTAGLIONE, Aureliano

Presenter: SCHULZ, Michael

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **79** Type: **Poster**

User experience: The upcoming user portal

Friday, December 9, 2022 3:30 PM (1h 30m)

As the demand for better and FAIR handling of generated data increase, we are implementing a new user portal that will provide:

- Data catalog with metadata about the collect datasets
- Data evaluation platform
- New Single-sign-on system

Primary authors: PEDERSEN, Bjoern (FRM II, TU München); FELDER, Christian; LOHSTROH, Wiebke

Presenter: PEDERSEN, Bjoern (FRM II, TU München)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

Status and Upgrades of the Instruments and the Positron Beam Facility at NEPOMUC

Friday, December 9, 2022 4:35 PM (25 minutes)

The bright low-energy positron beam provided by the neutron induced positron source in Munich (NEPOMUC) at FRM II is used in a large variety of experiments in materials science, condensed matter and surface physics as well as in fundamental research, e.g., for the creation of a positron-electron pair plasma. Within this contribution, an overview of the current status and developments of the positron beam facility with its instrumentation is given. Plans for the installation of a buffer gas trap for the creation of high-density positron pulses as well ideas for increasing the performance of the remoderated positron bam are elucidated. The upgrades of the positron beam instruments (i) Coincident Doppler-Broadening Spectrometer (CDBS) using a scanning positron micro beam, (ii) instrument for the 2D measurement of the Angular Correlation of Annihilation Radiation (2D-ACAR), and (iii) the surface spectrometer are highlighted. Finally, the planned extension of the positron beam facility and the future operation of positron beam experiments in the experimental hall *East* are presented.

Primary author: HUGENSCHMIDT, Christoph

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Presenter: HUGENSCHMIDT, Christoph

Session Classification: Poster Session

Track Classification: Positrons

Contribution ID: **81** Type: **Poster**

Status Report of the MEPHISTO Beamline

Friday, December 9, 2022 3:30 PM (1h 30m)

The author will present the actual status of the work at the MEPHISTO beamline and the Helium cryoplant system.

Primary author: Dr KLENKE, Jens (FRM II)

Presenter: Dr KLENKE, Jens (FRM II)

Session Classification: Poster Session

Track Classification: Nuclear, Particle and Astrophysics

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

Anionic surfactant detection using polydiacetylene-based nanocomposites

Friday, December 9, 2022 3:30 PM (1h 30m)

Polydiacetylenes (PDAs) are color-responsive polymers to various stimuli. The development of PDAs as anionic surfactant sensors by structural modification involved complicated and costly processes. In this study, we introduce a facile approach for preparing polydiacetylene/zinc (II) ion/zinc oxide (PDA/Zn2+/ZnO) nanocomposites utilized for anionic surfactant detection. Cationic surfactant, cetyltrimethylammonium bromide (CTAB) is incorporated into the nanocomposites via a simple mixing process to adjust their color transition behaviors. Addition of CTAB at 1 mM induces the blue-to-yellow color transition of the nanocomposites. Interestingly, the nanocomposites exhibit yellow-to-red color transition in response to sodium dodecyl sulfate (SDS). This demonstrates the ability of the nanocomposites as anionic surfactant sensors. A key mechanism of the color transition is the interaction between CTAB and SDS, which induces perturbation in the outer layers of the nanocomposites.

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Presenter: Mr YIMKAEW, Watsapon (Laboratory of Advanced Chromic Materials, Department of Materials Science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Status and perspectives of the neutron imaging instrument suite at MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

MLZ successfully operates the two neutron imaging beam lines NECTAR and ANTARES. NECTAR provides fast fission neutrons, thermal neutrons and gammas, which can be combined for multimodal characterization of larger samples with spatial resolution down to ~100 µm. ANTARES offers a spectrum with a thermal maximum, extended towards cold neutrons, providing higher sensitivity and spatial resolutions down to ~20 µm.
Many applications, such as studying the water management within membranes of fuel cells of only a few µm thickness or lithium transport phenomena and dendrite growth in batteries, require high spatial resolution for small samples combined with a high flux cold neutron spectrum. Moreover, many scientific questions requiring modern and advanced imaging techniques (e.g. grating interferometry, Bragg edge imaging) would strongly benefit from a broader spectral range and a colder spectrum.
We propose to build a complementary neutron imaging instrument at a neutron guide end position, providing a small beam cross section and a cold neutron spectrum combined with an extremely low background. The instrument will be optimized for applications requiring high spatial resolution down to the single µm range and applications using advanced imaging techniques that will benefit most from the broad spectral range and the low background at a neutron guide, adding world-wide unique capabilities to the portfolio of neutron imaging applications at MLZ.

Primary author: SCHULZ, Michael

Co-authors: SCHILLINGER, Burkhard; LOSKO, Adrian (Technische Universität München, Forschungs-Neutronenquelle MLZ (FRMII)); TARTAGLIONE, Aureliano (Technische Universität München, MLZ (FRM2))

Presenter: SCHULZ, Michael

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **84** Type: **Poster**

In situ study of superlattice self-assembly during slot-die coating of perovskite quantum dot films for solar cell applications

Friday, December 9, 2022 3:30 PM (1h 30m)

Research into quantum dots (QDs) of metal halide perovskites has become increasingly popular due to their stability and tunable optoelectronic properties. Their controllable surface chemistry and simple preparation make them a promising alternative to bulk perovskite solar cells. The power conversion efficiency (PCE) of $Cs_xFA_{1-x}PbI_3$ QD solar cells (QDSCs) has been steadily rising, up to a recent record efficiency surpassing 16%. However, the orientation and self-assembly of the colloidal precursor into a superstructure is not yet well-understood. In this work, we study the formation of perovskite QD films using in situ grazing-incidence X-ray scattering (GIXS), to achieve a better understanding of the kinetics involved in their fabrication.

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Co-authors: REUS, Manuel (TUM E13); MÜLLER-BUSCHBAUM, Peter (Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany; MLZ, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: KOSBAHN, David (TUM E13)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **85** Type: **Poster**

The small-angle scattering instrument SANS-1 at MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

We present the features of the instrument SANS-1 at MLZ, a joint TUM and Hereon project [1]. SANS-1 features two velocity selectors and a TISANE chopper, efficiently allowing to tune flux, resolution, duty cycle and frame overlap, including time resolved measurements with repetition rates up to 10 kHz.
A second key feature is the large accessible Q-range facilitated by the sideways movement of the primary $1m^2$ detector. Particular attention is hence paid to effects like tube shadowing and anisotropic solid angle corrections that arise due to large scattering angles on an array of single ^{3}He tubes, where a standard solid angle correction is no longer valid.
SANS-1 features a flexible, spacious sample stage equipped with a heavy-duty 1-ton goniometer, allowing hosting a wide range of different sample environment like a set of sample changers, magnets, ovens, a bespoke dilatometer for in-situ rapid quenching/heating and stress analysis [2] and a dedicated HF-coil system for nanomagnetic hyperthermia [3].
We show scientific highlights and current developments, e.g. a high T furnace that works as an insert for the 2.5T magnet, a future high field magnet and a pressure cell for GISANS. We also present the upgrade plans for a second detector array and a changed guide concept for a massive Q-range extension.

[1] S. Mühlbauer et al., NIMA 832, 297-305, (2016)
[2] TA Instruments, DIL805A/D/T Quenching dilatometer
[3] NB Nanoscale, D5 HF-Generator for Magnetic Hyperthermie

Primary authors: MUEHLBAUER, Sebastian; HEINEMANN, Andre (Hereon); Dr BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany); ALFALOU, Abdel; WILHELM, Andreas; VAGIAS, Apostolos (FRM2 / TUM); DEMBSKI-VILLALTA, Michal; SOLIS, Cecilia

Presenter: MUEHLBAUER, Sebastian

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **86** Type: **Poster**

Design, fabrication and nano-scale characterization of novel SEI layers

Friday, December 9, 2022 3:30 PM (1h 30m)

Lithium has a high specific capacity of 3860 mAh g−1 and a low electrochemical potential (-3.04 V), promising a high energy density lithium metal battery (LMB). However, the growth of lithium dendrites during charging and discharging would penetrate the separators in LMBs, which leads to short circuit. To inhibit the growth of lithium dendrites, we focus on optimizing the SEI layer through localized iodination for an interface and ion modulation. In the standard electrolyte (propylene carbonate/fluoroethylene carbonate/dimethyl carbonate=7.5/2/0.5 v/v/v, 1.05 M lithium bis(trifluoromethanesulfonyl)imide), a small amount of additive (poly (N-vinylimidazole) quaternized with iodide, molecular weight 16500 g/mol, 21% quaternization, abbreviated as PVIM) is added. We probe the electrochemical performance and morphology via Galvanostatic tests and scanning electron microscopy. Compared the control sample, Li-Li symmetrical cells with the PVIM additive electrolyte display a better electrochemical performance with smoother surface of lithium metal.

Primary authors: XU, Zhuijun (Technische Universität München); Prof. CHENG, Yajun (Ningbo Institute of Materials Technology and Engineering); Prof. XIA, Yonggao (Ningbo Institute of Materials Technology and Engineering); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: XU, Zhuijun (Technische Universität München)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **87** Type: **Poster**

Co-nonsolvency-Triggered Contraction of Poly(sulfobetaine)-based Diblock Copolymer Thin Films in Water/Acetone Atmosphere

Friday, December 9, 2022 3:30 PM (1h 30m)

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich and solvent-rich phase in a certain range of compositions of these two solvents. The nonionic thermo-responsive polymer, poly(N-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 mixtures by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier transform infrared (FT-IR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which is closely related to their deuteration level.

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

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **88** Type: **Talk (20 min + 5 min discussion)**

Clamp Cells for Neutron Scattering at the MLZ

Thursday, December 8, 2022 1:40 PM (25 minutes)

Clamp cells optimized for neutron scattering at low temperatures on the instruments DNS, MIRA, HEiDi, and POLI at the Heinz Maier-Leibnitz Zentrum [1] will be presented. The monobloc cell is available in two variants made of a CuBe alloy and a NiCrAl alloy, operational up to about 1.1 GPa and 1.5 GPa, respectively. Measurements aimed to elucidate magnetic properties are now possible due to the low paramagnetic moment of both alloys.
Tests with neutron radiation were performed to calibrate the load/pressure curve of the CuBe cell, to estimate its neutron absorption and background, and to measure magnetic reflections. In addition, the thermal response of the cells in the instrument cryostat was measured and the experimental findings were complemented by simulations.
A modified version of the cell with the same mechanical properties was developed with an optical access to the inner part of the cell, which enables the use of ruby luminescence to determine the pressure independent from neutrons. The respective load/pressure calibration curves were measured for both cell variants.
These cells are intended for high-pressure measurements on different instruments at MLZ suitable for all available magnets and cryostats down to 1.5 K.
[1] Eich A et al., High Press. Res., 41[1], 88–96 (2021)

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Presenter: GRZECHNIK, Andrzej (Jülich Centre for Neutron Science-4)

Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

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

A newly developed 100 KN testing machine optimized for in-situ microstructural characterization of high-temperature alloys

Friday, December 9, 2022 3:30 PM (1h 30m)

An innovative 100KN testing machine for, tensile, compression, and fatigue testing of industrially relevant high-temperature alloys has been developed and optimized for in-situ microstructural characterization of high-temperature alloys under mechanical and thermal loading. Moreover, this machine can be used as a new sample environment for in-situ experiments at FRM II, e.g., at the instruments Stress-Spec, Spodi, and SANS-1. Neutron Diffraction (ND) is performed to determine the lattice constants (misfit), phase fractions, and strain while Small-Angle Neutron Scattering (SANS) is applied to identify the size and the volume fraction of nano-sized γ´ precipitates. Deformation and heating, to simulate the application conditions, is performed in situ to determine the behavior of the alloy. It is possible to investigate the alloys at temperatures up to 1200 ℃ and with a maximum deformation of approximately 50%. A laser heating and an active cooling device are two developments for the testing machine in future.

Primary author: SARWAT, Faryal

Co-authors: NITSCHKE, Alexender (TUM); FRITTON, Massimo; GILLES, Ralph

Presenter: SARWAT, Faryal

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **90** Type: **Poster**

MIASANS at the longitudinal neutron resonant spin echo spectrometer RESEDA

Friday, December 9, 2022 3:30 PM (1h 30m)

The RESEDA (Resonant Spin-Echo for Diverse Applications) instrument has been optimized for neutron scattering measurements of quasi-elastic and inelastic processes over a wide parameter range. One spectrometer arm of RESEDA is configured for the MIEZE (Modulation of Intensity with Zero Effort) technique, where the measured signal is an oscillation in neutron intensity over time prepared by two precisely tuned radio-frequency (RF) flippers. With MIEZE, all of the spin-manipulations are performed before the beam reaches the sample, and thus the signal from sample scattering is not disrupted by any depolarizing conditions there (i.e. magnetic materials and fields). The MIEZE spectrometer is being further optimized for the requirements of small-angle neutron scattering (MIASANS), a versatile combination of the spatial and dynamical resolving power of both techniques. We present the current status of (i) newly installed superconducting solenoids as part of the RF flippers to significantly extend the dynamic range (ii) development and installation of a new detector on a translation stage within a new larger SANS-type vacuum vessel for flexibility with angular coverage and resolution, and (iii) efforts to reduce background.

Primary authors: LEINER, Jonathan (Technical University of Munich); FRANZ, Christian; JOCHUM, Johanna K.; PFLEIDERER, Christian

Presenter: LEINER, Jonathan (Technical University of Munich)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

Design, fabrication and application of PEO-based solid polymer electrolytes for all-solid-state lithium batteries

Friday, December 9, 2022 3:30 PM (1h 30m)

All-solid-state lithium batteries (ASSLBs) have received extensive attention as one of the most promising power sources for flexible and wearable electronics, mainly because of their high flexibility, high energy density and reliable safety. However, the practical application of ASSLBs has been hindered by the poor interfacial stability and inferior ionic conductivity. Therefore, the exploration of advanced solid electrolytes with superior interfacial compatibility/ionic conductivity is an important research topic for all-solid-state batteries. Solid polymer electrolytes (SPEs) exhibit great potential in developing solid-state batteries, specifically for PEO and PEO-based derivatives, because of their superior interfacial compatibility, outstanding solubility against lithium salts, wide electrochemical windows and high ionic conductivity. At the same time, solid fillers, as an important component in SPEs, play a crucial role in determining the overall electrochemical properties. As a consequence, we start from PEO-based materials and prepare SPEs by adding plastic additives and solid fillers with good structure. The electrochemical performance and structural stability of SPEs are elucidated by a combination of electrochemical characterization and morphological structural characterization.

Primary authors: YAN, Yingying (Lehrstuhl für Funktionelle Materialien, Physik-Department, TU München); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

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Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **92** Type: **Poster**

Morphology tuning of polymer templated Si/Ge/C anodes in Li-ion batteries

Friday, December 9, 2022 3:30 PM (1h 30m)

With high energy density, long lifespan, and environmental friendliness, lithium-ion batteries (LIBs) represent one of the most attractive energy storage devices and are playing increasing roles in modern society. This technology is already present in the portable electronics markets, electric vehicles, and small-scale energy storage systems. For higher performances, changing the anode material from graphite to silicon (Si) or germanium (Ge) could enhance the capacity multiple times. In particular, Si is a potential anode material due to environmentally friendly production, resource abundance, low cost and its outstanding high theoretical capacity of 4200 mAh/g (roughly ten times larger than state-of-the-art graphite). Although Ge has non-negligible drawbacks such as commodity price and abundance, it benchmarks Si and graphite in conductivity and Li+ diffusivity.

Our concept is to synthesize porous SiGe thin-films in a sol-gel approach via an amphiphilic diblock copolymer. In this process, polystyrene-b-polyethylene oxide (PS-b-PEO) acts as the structure-directing agent. As a Si/Ge source, soluble ZIntl-phases are used, where the amount of Si and Ge can be adjusted at your own discretion. These phases are polyanionic cages formed in intermetallic compounds between alkali or alkaline earth metals and p-block semimetals.

This work investigates the morphology-dependent battery performance of these Si/Ge/C thin films.

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Presenter: WEINDL, Christian (TUM Physik)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **93** Type: **Talk (20 min + 5 min discussion)**

Opportunities for P-wave Resonance Spectroscopy for Studies of Parity and Time Reversal Violation on POL

Thursday, December 8, 2022 2:05 PM (25 minutes)

The NOPTREX collaboration performs neutron spectroscopy measurements on p-wave resonances to quantify P-odd/T-odd measurement sensitivity. Beam-port adaptations to POLI would enable one of the highest fluxes of polarized eV neutrons in the world aided by the new 3He polarizer and analyzer. The 139La 0.7 eV p-wave resonance amplifies both parity-odd (P) and time-reversal odd (T) effects from mixing of s-wave and p-wave resonances [1], and a sensitive null test of T is possible for this observable [2]. Examples of correlations that can be measured on POLI for NOPTREX include (1) the P-odd correlation term A from k ·I in the forward scattering amplitude, where k is the neutron momentum and I is the nuclear polarization, (2) the pseudomagnetic precession term B from σ ·I, where σ is the neutron polarization. POLI can improve the precision of the only 139 La A measurement of A = 0.31 ± 0.09 [3] by 10x. The pseudomagnetic precession term σ ·I has never been measured on the 0.7 eV 139La resonance and would provide important information on systematics in the null test of T. POLI can enable these measurements others on p-wave resonances in 131Xe and 81Br for example. Proposals for the two experiments on 139 mentioned above will be detailed. This work is supported by NSF grant PHY-1913789.
[1] V. P. Gudkov, Physics Reports **212** 77 (1992).
[2] J. D. Bowman and V. P. Gudkov, Phys. Rev. C **90** 065503 (2014).
[3] V. P. Alfimenkov et al, Phys. Atm. Nucl. **59**, 1861 (1996).

Primary author: SNOW, W. Michael (Indiana University Bloomington)

Co-authors: BABCOCK, Earl; Mr OTERO MUNOZ, Gabriel (Indiana University Bloomington)

Presenter: BABCOCK, Earl

Session Classification: Nuclear, Particle and Astrophysics

Track Classification: Nuclear, Particle and Astrophysics

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

The direct geometry cold chopper spectrometer TOFTOF

Friday, December 9, 2022 3:30 PM (1h 30m)

TOFTOF is a direct geometry disc-chopper time-of-flight spectrometer. A cascade of seven fast rotating disc choppers is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging super-mirror section. The scattered neutrons are detected by 1000 3He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 12 m2 (or 0.75 sr). The high rotation speed of the chopper system together with a high neutron flux in the wavelength range of 1.4 -14 Å allows free tuning of the energy resolution between 3 meV and 2 μeV.
The fast neutron background is suppressed by the s-shaped primary neutron guide. This enables the investigation of weak signals. The existing linearly tapered neutron guide yields a beam spot size of 23x47 mm2. As alternative option a focussing guide can be used. This leads to an intensity gain up to a factor of 3 (wavelength dependent) on a sample area of 10 x 10 mm2.

TOFTOF represents a versatile instrument combining high energy resolution, high neutron flux (also at short wavelengths), and an excellent signal-to-background ratio. It is perfectly suited for inelastic and quasielastic neutron scattering for a broad range of scientific topics.

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Co-authors: GARVEY, Christopher (MLZ); LOHSTROH, Wiebke

Presenter: WOLF, Marcell (TUM)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

New options on the polarized neutron single crystal diffractometer POLI at MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

Polarized neutron diffraction is a powerful tool for studying condensed matter physics and to probe the spin and orbital properties of unpaired electrons. POLI is a polarized neutron single crystal diffractometer built on the hot neutron source at MLZ. Currently three standard setups are implemented on POLI: 1) zero-field spherical neutron polarimetry using CRYOPAD; 2) polarized neutron diffraction in magnetic fields; 3) non-polarized diffraction under various conditions.
We recently implemented a new actively shielded asymmetric split-coil superconducting magnet with a maximal field of 8T. The magnet is designed to facilitate polarized neutron diffraction with low stray fields, a large opening (3$\mathring{0}$ vertical) and a large sample space suitable for e.g., piezo goniometers and pressure cells. We also built a compact-size solid-state supermirror bender polarizer optimized for short neutron wavelengths to provide high neutron polarization in the vicinity of the magnet. An in-situ SEOP polarizer and analyzer will be available in 2023 which maintains high levels of neutron polarization and intensity over long periods of time. The SEOP polarizer are well shielded magnetically and can be used with the large magnet. Transferring the BIDIM26 area detector of size 26cm by 26cm from LLB to MLZ is in progress [3].

[1] V. Hutanu, J. Large-Scale Res. Facil. 1, A16 (2015).
[2] V. Hutanu et al., IEEE Trans. Magn. 58, no. 2, pp. 1-5, (2022).
[3] A. Gukasov et al., Physica B 397, 131 (2007).

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Presenter: Dr XU, Jianhui (RWTH Aachen University; Forschungszentrum Jülich GmbH)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **96** Type: **Poster**

The Macromolecular Neutron Single Crystal Diffractometer BIODIFF for Proteins at the Heinz Maier-Leibnitz Zentrum

Friday, December 9, 2022 3:30 PM (1h 30m)

Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules. At the FRM II neutron source the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is dedicated to the structure determination of enzymes. Typical scientific questions address the determination of protonation states of amino acid side chains, the orientation of individual water molecules and the characterization of the hydrogen bonding network between the enzyme active center and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behavior of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal. Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Recently a hexapod has been installed at BIODIFF which allows an online collimator alignment. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography. In addition, a potential detector upgrade will be presented.

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Presenter: OSTERMANN, Andreas (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

Session Classification: Poster Session

Track Classification: Structure Research

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

Tuning PNIPMAM Thin Films for Application as Humidity Sensors: The Influence of Salt Addition

Friday, December 9, 2022 3:30 PM (1h 30m)

Stimuli responsive polymers have gained much attention due to their unique properties. If polymer thin films exhibit a reversible volume change upon exposure to external stimuli such as temperature, pH, or solvents, they become promising candidates for applications such as nanoswitches or sensors. Polymers like poly(N-isopropyl methacrylamide) (PNIPMAM), which are sensitive to two stimuli can be used as bisensitive devices. PNIPMAM is a LCST-type thermoresponsive polymer and absorbs water molecules when it is exposed to water rich atmospheres. Due to low swelling times and strong volume changes upon water incorporation PNIPMAM thin films are of special interest. In this work, the influence of two different magnesium salts on the swelling behavior of PNIPMAM thin films is explored. In situ time-of-flight neutron reflectometry (ToF-NR) measurements are performed to investigate the macroscopic swelling behavior of the salt containing polymer thin films. By fitting the obtained reflectivity patterns, information about the distribution of the compounds vertically through the thin films can be deduced. To gain further insights on a molecular level and to understand the underlying hydration mechanism, additional in situ Fourier-transform infrared spectroscopy (FTIR) measurements are performed. Our studies showed, that the addition of different salts highly influences the swelling behavior as well as the hydration mechanism of PNIPMAM thin films depending on the salt additive.

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Presenter: REITENBACH, Julija (Technical University of Munich, Chair of Functional Materials)

Session Classification: Poster Session

Track Classification: Soft Matter

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

Use of High-concentration Lithium-ion Electrolyte to Overcome Challenges of High-temperature Lithium Batteries

Friday, December 9, 2022 3:30 PM (1h 30m)

Lithium secondary batteries (LSBs) have witnessed explosive growth in the last decade. Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. Herein, we demonstrate a new electrolyte that achieves an excellent stable long-term cycling at 100℃, well beyond the typical 60℃ limits of normal conventional Li-ion batteries. The high concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte promotes the formation of a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells. Moreover, it achieves reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) > 99.3%. Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by molecular dynamics (MD) simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes for Li-ion batteries.

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Presenter: ZHENG, Tianle (Technische Universität München)

Session Classification: Poster Session

Track Classification: Material Science

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

Capabilities in the upgraded MLZ Physics Lab

Friday, December 9, 2022 3:30 PM (1h 30m)

In this contribution, we present the new devices of the Physics Lab, which is open for all MLZ users. It comprises of a magnitude of different preparation and analytical tools, which are intended to support users for upcoming neutron scattering experiments. For analytical purposes, the lab offers the ability to use a digital microscope, x-ray reflectometer, x-ray residual stress diffractometer, a multi-purpose x-ray diffractometer and a DynaCool14 Physical Property Measurement System with dilution insert. The DynaCool14 has options for heat capacity, vibrating sample magnetometry, ac/dc resistance, ac susceptibility and much more. The XRDs allow to measure nearly all kind of samples, ranging from powders and solids to thin films and capillaries in order to conduct phase identification and quantification or investigation of film thickness and density. As sample preparation devices we are equipped with saws, polishers, powder grinders and high temperature ovens with inert gas.

Primary authors: Dr BOOK, Alexander (TUM); Mrs KENNEL, Teodora (TUM)

Co-authors: Dr SKOULATOS, Markos (TUM); Mr WAURO, Matthias (TUM)

Presenter: Dr BOOK, Alexander (TUM)

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **100** Type: **Talk (20 min + 5 min discussion)**

How Neutrons and X-rays Help Us Understand Electrochemistry

Thursday, December 8, 2022 3:00 PM (25 minutes)

Electrochemistry –especially within the context of energy storage, has become a key element of society. Understanding its processes is essential, e.g., for the making of cheaper, lighter and safer batteries or the synthesis of novel functional materials. A number of the concerned processes takes place at so-called "buried-interphases", which can only be investigated using advanced characterization techniques with high penetration depth and sensitivity. This is the case for neutrons and high energy x-rays, which can hence be used to unravel reactions and mechanisms whilst ongoing. Small-angle scattering allows for the detection of structural changes from a couple to a few hundreds of nanometers with high statistical relevance due to high probe flux and relatively large sample area. Small-Angle Neutron Scattering was applied to follow the morphology of a single-ion polymer electrolyte inside a lithium metal cell during cycling at high temperature, which revealed the structural stability of the material under harsh conditions. When used in reflection geometry, Grazing Incidence Small-Angle X-ray Scattering can be used to determine the average structure of thin films, which was done for the case of electrochemically deposited mesoporous silica films. This revealed the vertically oriented hexagonal structure of the porous network and led to the finding of an aggregate-free deposition protocol. This shows the versatility of neutron and X-ray techniques towards new technologies.

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Presenter: MOEHL, Gilles (ADVMAT)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **101** Type: **Poster**

Fabrication and Characterisation of Two-Step Slot-Die Coated Methylammonium-Formamidinium Lead Iodide Perovskite Solar Cells

Friday, December 9, 2022 3:30 PM (1h 30m)

Perovskite solar cells (PSCs) are very promising in contributing in the renewable energy mix of the future. They have high power conversion efficiencies and are made of low-cost materials. Especially in combination with slot-die coating as promising thin-film deposition technique for organic-inorganic hybrid perovskite materials, they offer the chance for a fast and cheap roll-to-roll solar cell production.
In this work two-step slot-die coated lead iodide layers and slot-die coated methylammonium-formamidinium iodide perovskite solar cells have been prepared. Depending on slot-die coating parameters and additives used in the γ-butyrolactone (GBL) containing ink that enhance thin-film formation and optoelectronic properties of the final perovskite semiconductor absorber, morphology changes are observed in the final film. The morphology is investigated by reciprocal (X-ray diffraction) and real-space methods (SEM). Furthermore, the two-step slot-die coated solar cells are produced and characterized via their respective performance parameters.

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Presenter: BAIER, Thomas

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **102** Type: **Poster**

Magnetic Wollaston Prisms for spatial intensity modulations of polarized neutron beams at FRM II

Friday, December 9, 2022 3:30 PM (1h 30m)

The MIEZE (Modulated IntEnsity with Zero Effort) resonant spin-echo technique at the RESEDA instrument at FRM II has its optimum resolution at small scattering angles, i.e. SANS type geometries. Recent upgrades (MIASANS) have further increased the resolution in the small angle regime. Going forward, there is the possibility [1] to extend the optimum MIEZE resolution to wide angles by incorporating superconducting magnetic Wollaston prisms (MWPs) into the beamline. These MWPs will produce controlled spatially intensity modulations in addition to the intensity modulations in time inherent to MIEZE. The resultant capability to make corrections to the neutron time of flight allows for the systematic spatial focusing of the MIEZE resolution function to any desired scattering angle. Additionally, MWPs will be useful in the context of intra-particle mode-entangled neutron beams for potential use in probing many-body quantum entanglement in materials. Finally, the compact and modular nature of the MWPs will allow them to be used to measure diffraction peaks with enhanced resolution at several polarized beam instruments such as MIRA, KOMPASS, LaDiff, and in general at small angle neutron scattering instruments. We present the plans for the construction of these superconducting MWPs for use at FRM II, and describe the details of their operation and the various possibilities they offer.

[1] Fankang Li, J. Appl. Cryst. **55**, 90-97 (2022).

Primary authors: METTUS, Denis (Technische Universität München); LEINER, Jonathan (Technical University of Munich); JOCHUM, Johanna K.; PFLEIDERER, Christian

Presenter: METTUS, Denis (Technische Universität München)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **103** Type: **Poster**

Analysis of certified reference alloys using PGAA and in-beam NAA methods

Friday, December 9, 2022 3:30 PM (1h 30m)

Neutron-based analytical techniques (such as prompt gamma activation analysis and neutron activation analysis) are preferred in the non-destructive bulk analysis of archaeological objects, modern alloys with protective layer, and in case of materials containing elements that are insoluble for destructive quantitative analysis. Both nuclear analytical techniques are primary methods of measurement playing an important role in analytical chemistry. Reference alloys were analyzed with PGAA and NAA in the BNC, and further PGAA and in-beam NAA experiments were carried out on them at MLZ. The combination of PGAA and in-beam NAA was the most effective to determine the alloy components, their results were in good agreement with the reference values. As, Sb and Mn had the best detection limits (tens of ppm) with in-beam NAA. Zn was detectable in ppm level only with NAA. The detection limit of Pb, an important component of bronzes is 1.7-3.0 mass percent in the presence of the dominant copper. An emerging technique, fast neutron PGAA based on the inelastic neutron scattering offers higher sensitivities for several elements of interest, than cold-neutron PGAA, as the cross sections for the fast neutron reactions are similar for every element (0.1-10 barn). This makes possible the analysis of materials containing heavy elements (like Pb) even when thick samples are used. We plan to continue the analyses of reference materials using fast neutron PGAA at the FaNGaS facility at the MLZ.

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Presenter: MARÓTI, Boglárka (Centre for Energy Research)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **104** Type: **Talk (20 min + 5 min discussion)**

In-situ neutron diffraction study of Ni-addition influence on phase transformations in Co-Re-Cr high-temperature alloys

Thursday, December 8, 2022 3:25 PM (25 minutes)

Among new alloy systems being developed to supplement Ni-based superalloys in gas turbine applications, the Co-Re-based alloys show promise because of their excellent specific strength and relatively high melting range (1490°-1560℃). Alloying elements with various functions are added to these alloys. For example, Cr, and Ni, for oxidation resistance. Since the Co matrix undergoes an allotropic transformation from the low-temperature closed packed hexagonal structure to the high-temperature face-centred cubic structure, a two-phase matrix exists in Co-Re alloys at intermediate temperatures. Moreover, Cr addition above 20 at.%, however, pose a challenge – namely the formation of topologically closed packed Cr2Re3-type σ-phase. It is generally avoided in high-temperature alloys as its presence causes brittleness. The Co-Re alloys designed at TU Braunschweig are now being investigated for improving oxidation resistance and, simultaneously, suppression of σ-phase. It is intended to achieve this goal by a partial replacement of Cr with Ni atoms.
To fully reveal changes in bulky polycrystalline samples over the whole volume, in-situ neutron diffraction measurements were performed during heating to high temperatures and cooling for various Ni and Cr content alloys. The allotropic transformation of the Co-matrix and the evolution of the low-temperature hexagonal and high-temperature cubic Co phases were studied, and a phase diagram for this complex system was constructed.

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Presenter: BERAN, Premysl (Nuclear Physics Institute CAS)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **105** Type: **Poster**

3He polarization group at the JCNS

Friday, December 9, 2022 3:30 PM (1h 30m)

The 3He group has developed in-situ polarizers for many JCNS instruments including MARIA, TOPAS, KWS1, POLI, and KWS2 and will provide another two polarizers for the ESS for DREAM and TREX. We develop all 3He cells and magnetic systems in house, as well as the laser sources for the FRM2-based devices. We have also work towards wide angle analysis with C-shaped analyzer cell. The status and concepts of the various installations will be discussed.

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Presenters: BABCOCK, Earl; SALHI, zahir (JCNS)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **106** Type: **Poster**

ENHANCED AIR STABILITY OF GREEN-SOLVENT POLYMER SOLAR CELLS WITH GREEN-FLUORESCENT POLYMER

Friday, December 9, 2022 3:30 PM (1h 30m)

The performance of polymer solar cells (PSC) underwent a great development due to material design and device engineering, while the poor stability of PSCs and the use of toxic solvents during device fabrication are the most two big challenges nowadays hindering a large scale application. Here, we select a green-solvent based material system PBDB-TF-T1:BTP-4F-12 as our research model, and explore a green fluorescent polymer additive EH-P that improves the air-illumination stability of these solar cells without too serious effects on the device performance. Thereby, this work demonstrates great potential in the real application of polymer solar cells.

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Presenter: LI, ZERUI (TUM)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **107** Type: **Poster**

PUMA: Thermal neutron three axes spectrometer

Friday, December 9, 2022 3:30 PM (1h 30m)

Thermal neutron three axes spectrometer PUMA is characterized by a very high neutron flux as a result of the efficient use of focusing techniques. An innovative option of the spectrometer is the multianalyzer/detector system, which allows a unique and flexible type of multiplexing. Using this option, a scattering angle range of 16° can be measured simultaneously and flexible Q-ω paths can be realized without repositioning the instrument. The typical scientific applications of PUMA are studies of phonons and magnons. Furthermore, a unique feature of the instrument is the possibility to perform stroboscopic, time resolved measurements of both elastic and inelastic signals on time scales down to the microsecond regime. Using this technique, the sample is periodically perturbed by an external variable such as temperature, electric field, etc. The signal is then recorded not only as a function of momentum and energy transfer, but also given a time stamp, relative to the periodic perturbation. Since 2021, the Neutron Scattering Group of the Institute of Quantum Materials and Technologies (IQMT, www.iqmt.kit.edu) of the Karlsruhe Institute of Technology (KIT) has been jointly operating the PUMA three-axes spectrometer at MLZ within the framework of a collaboration contract. The purpose of the collaboration is to promote the scientific program, support the user program and develop instrumental capabilities.

Primary authors: GAZIZULINA, Alsu; MAITY, Avishek; WEBER, Frank (Karlsruhe Institute of Technology); PARK, Jitae

Presenter: GAZIZULINA, Alsu

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **108** Type: **Poster**

Volumetric and Localized Annihilation Signatures of a Magnetically Confined Electron-Positron Pair Plasma

Friday, December 9, 2022 3:30 PM (1h 30m)

The APEX collaboration aims to magnetically confine electron-positron pair plasma and diagnose the plasma with FPGA-processing of annihilation detections from an array of 48 Bismuth-Germanate (BGO) scintillators. Direct annihilation of pairs and the annihilation of positronium (Ps), formed through radiative and three-body recombination produce a volumetric source of gammas. Back-to-back two-gammas from direct or para-Ps annihilation can be detected in coincidence, allowing for tomographic reconstruction of the volumetric source. Three-photon decay, on the other hand, signifies the self-annihilation of ortho-Ps. Ionization of drifting Ps and collisions with neutrals and charged particles drive cross-field transport, which results in localized sources of two-gamma annihilation at the wall and magnet. The rates of the various annihilation mechanisms depend on the plasma temperature and density and the partial pressures of background gases. Triangulation, distance-attenuated single-photon counting, and the ratio between localized and volumetric decays will provide diagnostics for the properties and evolution of the plasma. We are developing techniques to differentiate between volumetric and localized gamma-ray sources and have conducted measurements with β+ emitters placed on rotating turntables to emulate pair plasma
distributions.

Supported by the Alexander von Humboldt Foundation, ERC (ERC-2016-ADG No. 741322), DFG, and U. S. DOE (DE-SC0019271).

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Session Classification: Poster Session

Track Classification: Positrons

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

Ionic liquids tailoring crystal orientation and electronic properties for stable and high fill factor perovskite solar cells

Friday, December 9, 2022 3:30 PM (1h 30m)

The crystallization behavior of metal halide perovskite thin films has a profound influence on the resulting defect densities, charge carrier properties and photovoltaic performance characteristics. Herein, we introduce a pyrrolidinium-based ionic compound (Pyr14BF4) into the perovskite to investigate the impact of ionic liquids on the crystal growth of perovskite films. Using time-resolved measurements, we probe the charge generation, transport and recombination behavior in these films and related devices. We find that ionic liquids can tailor the crystal growth from a disordered to a preferential corner-up orientation during film formation and accordingly increase the charge carrier mobility to accelerate electron transport and extraction. The highest power conversion efficiency achieved based on ionic liquid-containing devices is up to 21.49% and is accompanied by a high fill factor of 0.87. Via operando grazing-incidence small- and wide-angle X-ray scattering measurements, we observe a light-induced lattice compression and grain fragmentation in the control devices, whereas the ionic liquid-containing devices exhibit a slight light-induced crystal reconstitution and stronger tolerance against illumination. Under ambient conditions, the non-encapsulated Pyr14BF4-containing device maintains 97 % of its initial efficiency after 4368 h. Our results reveal the crucial role of ionic liquids in perovskite crystallization, charge carrier kinetics and device stability.

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Session Classification: Poster Session

Track Classification: Material Science

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

MARIA –The high-intensity polarized neutron reflectometer of JCNS

Friday, December 9, 2022 2:00 PM (1h 30m)

The high-intensity reflectometer MARIA of JCNS, is installed in the neutron guide hall of the FRM-II reactor and is using a velocity selector (4.5Å<λ<40Å) with a resolution of 10%. By using Fermi-Chopper the wavelength resolution can be increased to 1% or 3%. The beam is polarized by a double-reflecting super mirror (4.5Å<λ<12Å) and in the vertical direction the elliptically focusing neutron guide increases the flux at the sample position reducing the required sample size or measuring time. A flexible Hexapod, as sample table, can be equipped with an electromagnet (up to 1.1T) or a cryomagnet (up to 5T), low temperature sample environment, a UHV-chamber (10^{-10} mbar range) for the measurement of Oxide MBE samples, and various soft matter solid/liquid interface cells connected to a "sample robot"for automatic solvent contrast exchange and remote controlled heating/cooling. Together with the 400x400 mm² position sensitive detector and a time-stable ³He polarization spin filter based on SEOP technique, the instrument is well suited for investigating specular reflectivity (up to 7-8 orders of magnitude), off-specular scattering from structures down to the monolayer regime. The GISANS option can be used to investigate lateral correlations in the nm range. Due to the large detector even grazing incidence diffraction measurements are possible. Furthermore the high intensity allows for kinetic measurements down to a few seconds over a dynamic range of 3-4 orders.

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Presenter: ZHERNENKOV, Kirill (Jülich Forschungszentrum GmbH)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **111** Type: **Poster**

Printing parameter optimisation of additively manufactured ER120S-G steel using neutron tomography

Friday, December 9, 2022 3:30 PM (1h 30m)

Additive Manufacturing (AM) has become a viable manufacturing technique, because of its remarkable ability to manufacture parts with intricate shapes and superior mechanical properties. Wire laser additive manufacturing (WLAM) is a kind of Direct Energy Deposition (DED) technology where a wire is fed through a nozzle and deposited onto a substrate and melted by focussing one or more laser beams onto it. This technique is especially advantageous for local repair as well as printing large and complex 3D parts. Like most AM techniques, this involves rapid heating and cooling of samples, leading to specific microstructures and defects, which are influenced by both: the type of technique and the process parameters used. A proper characterization of these defects is imperative for optimal manufacturing process development.
In this work neutron tomography -performed at the NEUTRA instrument of SINQ (PSI, Switzerland) has been used to image the pores and defects in approximately cm-sized ER120S-G steel samples manufactured via Wire DED using three different printing strategies. These results have been linked with the assessment of the mechanical properties to arrive at suitable printing conditions. Additionally, different build strategies for the formation of complex shapes for this alloy have also been similarly characterized. The results from thermal neutron tomography will be duly presented.

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Presenter: KUMAR, Richi

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **112** Type: **Talk (20 min + 5 min discussion)**

A buffer-gas trap for the NEPOMUC positron beam

Thursday, December 8, 2022 5:10 PM (25 minutes)

Buffer-gas positron traps (BGT) are invaluable for high-resolution matter-antimatter interaction studies, antihydrogen research, and positronium laser spectroscopy. These devices exploit inelastic interactions between positrons and nitrogen molecules to accrue a nonneutral e^+ plasma [1]. We present plans to produce short pulses of very low-energy positrons by installing a BGT at the NEPOMUC positron facility [2].

A two-stage BGT and accumulator has been constructed at MPG-IPP to capture positrons from the 20-eV, remoderated NEPOMUC positron beam [3]. Testing of the traps with electron plasmas is underway. Potential applications for the NEPOMUC BGT include positron-annihilation-induced Auger-electron spectroscopy and production of a very dense positronium gas. Together with a high-field multicell trap [4], the BGT will be a crucial component of the APEX pair-plasma experiment [5], which requires an unprecedented number of low-energy positrons.

This work supported by European Research Council (ERC-2016-ADG No. 741322), U.S. DOE (DE-SC0019271), and the UCSD Foundation.

[1] Murphy, et al., Phys. Rev. A 46, 5696 (1992).
[2] Hugenschmidt, et al., New J. Phys. 14 055027 (2012)
[3] Stanja, et al., Nuc. Inst. Methods A 827, 52 (2016).
[4] Singer, et al., Rev. Sci. Inst. 92, 123504 (2021).
[5] Stoneking, et al., J. Plasma Phys. 86, 15586061 (2020).

Primary author: DELLER, Adam (IPP)

Presenter: DELLER, Adam (IPP)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **113** Type: **Talk (20 min + 5 min discussion)**

Parametrization of neutron instruments at MLZ

Thursday, December 8, 2022 4:15 PM (25 minutes)

Data obtained at a publicly funded research facility such as MLZ becomes available to other researchers after some period of time. The motivation for this policy is to make it possible to reuse data or verify published results. Given the huge variety of instruments, methods, and the extreme complexity of some of the experimental workflows, reuse of such data becomes absolutely impossible without proper and comprehensive documentation describing the available datasets. Each dataset must be attributed with a set of metadata needed for future analysis. Building such metadata schemas for each instrument and method is not possible without close collaboration with a competent and experienced instrument responsible scientist and user community. Here we demonstrate our attempts to assemble metadata sets describing data obtained by three fundamentally different neutron scattering instruments, such as triple-axis spectrometer, diffractometer and small-angle neutron scattering instrument. Despite significant differences in instrument design, measurement algorithms, and data structures, we are trying to unify the approach to constructing experiment metadata schemes.

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Session Classification: Neutron Methods

Track Classification: Neutron Methods

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

Upgrade of the KWS-2 SANS instrument for increased performance and beam-time efficiency

Friday, December 9, 2022 4:35 PM (25 minutes)

KWS-2 is a classical small angle neutron diffractometer where the pinhole mode with different neutron-wavelengths and detector distances can be combined with focusing mode with MgF2 lenses to reach a wide Q-range between 2x10-4 and 1 Å-1. Upgrades in the detection system and sample environment are currently in progress. A wide-angle detection option is currently in test and optimization and will enable measurements over an extended Q-range up to 2 Å-1, which will be beneficial for semi-crystalline materials and small biological morphologies. The high neutron flux determined the optimization of the measurement procedure for optimizing the beam-time use. A new versatile sample positioning system in beam including a thermostated multi-position carousel, robotics elements and a pool of sample cuvettes are currently in installation at the sample position of the instrument. This will enable the continuous supply of the instrument with samples and the possibility to schedule measurements on similar samples or effects in a common long experimental session. Finally, a new size exclusion chromatography setup with in-situ UV-Vis spectroscopy, is currently in construction for providing the instrument with samples of a desired quality, which will improve the performance of KWS-2 for studying aggregation prone proteins and will allow for highly individualized studies of biophysics and soft matter samples. The new upgrades in progress at the instrument will be presented in details.

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Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **115** Type: **Talk (20 min + 5 min discussion)**

Quantitative analysis and benchmarking of positional accuracy on neutron strain scanners – INTRODUCING THE NEUTRON QUALITY LABEL

Thursday, December 8, 2022 3:50 PM (25 minutes)

The neutron strain pilot projects within H2020- Sine2020 and BRIGHTNESS2 towards European neutron landscape & users have been key for facilitating industry access and collaborations in a regular basis. The shortcomings reducing the industrial experimental throughput are well known and very similar to all facilities. A central issue is the non-acceptance by industry to use the neutron technique as industrial standard. This "standardisation problem"addresses the urgent need of an established calibration method guaranteeing identical results for industry partners on different instruments at different facilities.
The proposed Neutron Quality Label stablishes common calibration samples and reporting addressing positional accuracies and comparison of software, hence promoting the exchangeability and sustainability of neutron strain characterization between participants.

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Presenter: CABEZA SANCHEZ, Sandra (ILL)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **116** Type: **Talk (20 min + 5 min discussion)**

LIMPID Applied to DBS Measurements on Multilayer Systems

Thursday, December 8, 2022 3:25 PM (25 minutes)

LIMPID (Layer-wise Investigation of Measurements on Positron Implantation and Diffusion) is a new analysis tool for positron depth profiles generated by variable energy Doppler-broadening spectroscopy. It allows the user to extract positron diffusion lengths by fitting the measured line-shape parameters as a function of implantation energy. The code is written in Python and open source, thereby 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. By taking into account sample properties such as mass density and composition, LIMPID can be used to determine other sample parameters like, e.g., layer thicknesses in multilayer systems. We demonstrate the main features of LIMPID using measurement data obtained from Cu/Cr bilayers on a Si substrate. Furthermore we discuss the performance of the code and compare it to VEPFIT, the current, albeit outdated, standard software.

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Presenter: MATHES, Lucian

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **117** Type: **Talk (20 min + 5 min discussion)**

SoNDe High-Flux Neutron Detector

Thursday, December 8, 2022 1:40 PM (25 minutes)

New high-flux and high-brilliance neutron sources demand a higher count-rate capability inneutron detectors. In order to achieve that goal, the Solid-State Neutron Detector (SoNDe)project developed a scintillation-based neutron detector. It is capable of fully exploiting theavailable flux current and coming neutron facilities, such as the European Spallation Source(ESS).[1] In addition to enabling high count-rates, one of the design goals was to develop amodular and scalable solution that can also be used in other instruments or differentcontexts, such as for laboratory setups.[2] Since higher brilliance and flux sources call for detectors that can handle high-flux,especially when considering pulsed sources with high peak-flux, SoNDe provides
-Possibility to handle a flux of more than 50 MHz on a 1x1 m^2 detector area
-Pixel resolution down to 3x3 mm^2
-Neutron detection efficiency higher than 80%, good gamma-discrimination
-µs time resolution
Count rates of 250 kHz per module (5 x 5 cm^2) were measured under primary beamconditions at neutron scattering experiments. Combined with the high area coverage of thesquare modules and the high efficiency of the scintillator this allows to use high flux neutronsources to capacity.
[1] JAKSCH, Sebastian, et al. Proceedings of the International Conference on NeutronOptics (NOP2017). 2018. S. 011019
[2] JAKSCH, Sebastian, et al. Cumulative Reports of the SoNDe Project July 2017. arXiv preprint arXiv:1707.08679, 2017

Primary authors: JAKSCH, Sebastian (Physicist); ENGELS, Ralf; DESERT, Sylvain (CEA Saclay - LLB); FRIELINGHAUS, Henrich (JCNS)

Presenter: JAKSCH, Sebastian (Physicist)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **118** Type: **Poster**

SKADI: Small-Angle Neutron Scattering at ESS

Friday, December 9, 2022 3:30 PM (1h 30m)

The Small-K Advanced DIffractometer (SKADI) is a joint in-kind project of French and German partners to deliver a SANS instrument to the ESS. [1,2] This contribution details the current construction status of SKADI. Further practical requirements on components such as the sample area will also be considered. SKADI is designed to deliver
-Flexibility (sample area is approx. 3x3 m^2, and versatile collimation)
-Very small Q accessible through VSANS
-Polarization for magnetic samples and incoherent background subtraction
-Good wavelength resolution, being the longest SANS instrument at ESS
-High dynamic Q-range over three orders of magnitude.
This will be combined with a neutron flux of 8E8 n/s cm2 at sample position, which will make it the world's brightest SANS instrument.
In addition to complex sample environments SKADI will also feature a newly developed detector system, SoNDe, developed within the EU Horizon2020 framework. [3]
SKADI caters for a wide range of scientific areas, such as smart materials, biological and medical research, magnetic materials, as well as experiments on nanomaterials and nanocomposites or colloidal systems. Finally, SKADI is designed to accommodate custom made sample environments to provide "real-world" conditions.
[1] JAKSCH, S., et al. NIMA, 2014, 762, p. 22-30.
[2] JAKSCH, S., et al. Appl. Sci., 2021, 11. , p. 3620.
[3] JAKSCH, S., et al. Proceedings of the International Conference on Neutron Optics (NOP2017). 2018. p. 011019.

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Presenter: JAKSCH, Sebastian (Physicist)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **119** Type: **Poster**

Overview on the Transformations in Austempered Ductile Iron

Friday, December 9, 2022 3:30 PM (1h 30m)

Austempered ductile iron (ADI) has undergone a special heat treatment to enhance mechanical properties. This heat treatment process consists of austenitization, quenching to a temperature between 250℃ and 450℃ and isothermal austempering, after which the microstructure consists of acicular ferrite and high carbon enriched retained austenite.
The high carbon enriched retained austenite can transform to martensite during plastic deformation. The treatment parameters (austenitization temperature, austempering temperature, austempering time and alloying composition) can influence the retained austenite fraction, grain size and its stabilization, which in turn will influence the following martensitic transformation.
The influence of different treatment and composition parameters on the martensitic transformation and texture formation during plastic deformation has been investigated using neutron and synchrotron diffraction. The combination of texture analysis and in-situ deformation tests allowed quantitative phase analysis and extraction of martensite phase fractions as a function of strain level.

In this presentation, we will give an overview of the current status of these experiments together with new results from recent atom probe tomography measurements.

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Presenter: HOELZEL, Markus

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **120** Type: **Talk (20 min + 5 min discussion)**

Spectroscopy data library for prompt gamma activation analysis

Thursday, December 8, 2022 5:10 PM (25 minutes)

The establishment of the spectroscopy data library for prompt gamma activation analysis (PGAA) was initiated 25 years ago, as no reliable (n,gamma) database existed for analytical purposes. The database lists partial cross sections and peak energies of elements used in chemical analysis. The first versions were published in [1], also in IAEA TECDOC, and has been used worldwide. More than 20,000 samples were successfully analyzed with it in our labs. The database has been continuously improved with targeted measurements.
The project was relaunched at the Garching reactor in 2011, where the beam is much stronger allowing for the use of thinner and smaller samples. Thus, the systematic errors from self-attenuation and random coincidences could be eliminated. The whole periodic table is being remeasured in elemental and compound form. Until the last cycle, the project reached about 80% completeness and it needs about 20 more beam days. Last year, the database had a major update: the ambiguous peaks have been deleted, many standardizations were improved based on measurements of high-quality stoichiometric compounds, which were not yet available 20–25 years ago. The evaluation is in progress. The final version is invited to be published in Atomic Data Nuclear Data Tables.
[1]Zs. Révay, R.B. Firestone, T. Belgya, G.L. Molnár: Prompt Gamma-ray Spectrum Catalog, in: Handbook of Prompt Gamma Activation Analysis with Neutron Beams, (G.L. Molnár ed.), Kluwer, Dordrecht, 2004, pp.173–364.

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Presenter: Dr REVAY, Zsolt (PGAA)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **121** Type: **Poster**

Design of a new model system for viral fusion

Friday, December 9, 2022 3:30 PM (1h 30m)

The fusion of viral and host cell membranes is a pivotal step in the infection and life cycle of any virus. The coronaviridae present a taxonomic family with a complex and highly diverse fusion behavior across different species and viral host environments. Despite the massive global research interest in SARS-CoV-2 many aspects of the fusion process are still only rudimentarily understood. Biological fusion assays are widely applied to study different steps of viral-host membrane fusion, however, multidisciplinary approaches offer a broader range of parameters to study. Here, we report the establishment of a new model system for viral fusion based on the neutron scattering behavior of tailored unilamellar lipid vesicles with specific membrane proteins.

Our target was to design individual vesicles from cellular material which only contain the membrane proteins included in the initial cellular plasma membrane and none of the organelle membranes within the cell. Thus, by protein expression on the cells, individual virion and target vesicles could be designed. The results of creating 100 nm unilamellar vesicles were confirmed by several methods, among the dynamic light scattering as well as small-angle X-ray and neutron scattering.

In order to investigate specific features of infection by vesicle fusion in the initial infection stages of SARS-CoV-2 this model system can be fitted with any viral or host cell membrane protein on the surface.

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Presenter: JAKSCH, Sebastian (Physicist)

Session Classification: Poster Session

Track Classification: Soft Matter

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

A Study of Lattice Defects in Tungsten using a slow Positron Beam

Friday, December 9, 2022 3:30 PM (1h 30m)

Predicting helium retention in tungsten is of relevance for future nuclear fusion reactors as it influences tritium uptake and transport, two processes which are critical factors in achieving 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 a "simple"system, i.e tungsten mono-crystals that only contain single vacancy defects.

We therefore compare samples where defects have been induced by either MeV electron bombardment or thermal quenching. While the initial and post damaging state of the samples is 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 which has been modified to deliver acceleration voltages of up to 40 kV.

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Presenter: BURWITZ, Vassily Vadimovitch

Session Classification: Poster Session

Track Classification: Positrons

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

Neutron Depth Profiling and X-Ray Diffraction to Study Lithiation Mechanism of LiAl Electrodes

Friday, December 9, 2022 3:30 PM (1h 30m)

Metal alloys, such as LiAl, are gaining more interest as anode materials for Li ion batteries because they exhibit a high theoretical capacity with 993 mAh/g while being inexpensive. During lithiation, aluminium begins to form a solid solution with Li, the so called alpha-LiAl phase. Once the solubility limit is reached upon lithiation, the alpha-LiAl undergoes a phase transition to the beta-LiAl phase.
Al electrodes were electrochemically lithiated to different state of charges in coin cells with Li metal as counter electrode. X-ray diffraction measurements were conducted on the disassembled anodes.The Rietveld refinements yield that the samples charged to SoC25 show a higher amount of alpha-LiAl. Simultaneously, the amount of beta-LiAl in the samples increases with higher SoC as expected.
Additional neutron depth profile measurements were performed in NPI CAS Rez at the CANAM infrastructure to determine the Li distribution throughout the lithiated samples. First results have confirmed that the lithiation of the aluminium starts at the surface where a higher Li concentration was identified. The higher charged sample also shows a stronger lithiation in the bulk of the Al anode. In the lower charged sample, no Li was detected near the backside of the anode, indicating that pristine Al is still present.
This work was performed as collaboration between TUM (FRM II) and RWTH Aachen (ISEA) in the frame of the BMBF project ExcellBattMat cluster.

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Presenter: PHAM, Thien An

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **124** Type: **Talk (20 min + 5 min discussion)**

Fractional Excitation-induced Phonon Renormalization in α-RuCl3

Thursday, December 8, 2022 3:25 PM (25 minutes)

The quantum spin liquid (QSL) phase is of immense interest to condensed matter physicists, and have been studied for decades. With a Kitaev model that is exactly solvable and gives a QSL ground state, α-RuCl3 is a promising Kitaev QSL candidate. Above the critical magnetic field Bc~7T and below T~6K there is evidence for the half-integer quantized plateau where anomalous measurements possibly arise from the fractional excitations in the QSL phase. Recent theoretical work has shown that the fractional excitations can induce phonon renormalization via the spin-lattice coupling, and would in particular affect the acoustic phonons, where longitudinal/transverse phonons harden/soften, respectively, as they approach the zone boundary. Our measurements have focused on the phonon dispersion in α-RuCl3 to observe this phonon renormalization effect in the putative QSL phase. We have used high-quality in-house grown α-RuCl3 single crystals for inelastic neutron and x-ray scattering measurements, combined with phonon dynamics calculations, to survey the acoustic phonons in the relevant scattering directions, in particular under magnetic fields. We will discuss our results with a focus on examining the low-energy acoustic phonon branches for the phonon renormalization effect.

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Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **125** Type: **Poster**

SAPHiR: Neutron science at high pressure and temperature conditions

Friday, December 9, 2022 3:30 PM (1h 30m)

SAPHiR, the Six Anvil Press for High Pressure Radiography and Diffraction, belongs to a suite of new instruments at the FRM II neutron source in Garching. The instrument will provide high pressure and temperature environments for in situ neutron measurements of powder samples, fluids, and melts. The pressure is generated by a cubic multi-anvil press, currently capable of reaching 15 GPa, with sample volumes of 10-50 mm3 and temperatures up to 2300 K. For neutron diffraction, SAPHiR employs the time-of-flight method, where scattered neutrons are measured with three position sensitive helium-3 detector banks and a wavelength-shifting-fibre scintillator detector system. Applications of SAPHiR include in situ crystallography and phase relations of light-element-bearing phases, equations of state, reaction kinetics, high-resolution radiography, and rheological studies. In addition to high-temperature conditions that are generated by an internal resistance furnace, samples can also be investigated below room temperature to ~80 K using a newly developed cryo-system. This system will be used for in situ studies of materials at low temperature, such as high-pressure ice phases, high-temperature super-conductors, and other materials science applications. The start of in situ neutron measurements and external user operation is currently projected for 2023; until that time, SAPHiR is being used offline for scientific studies.

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Presenters: HOWARD, Christopher (FRM II, TU München); WALTE, Nicolas (FRM II, TU München)

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **126** Type: **Poster**

Next generation asymmetric horizontal SANS magnet for quantum phenomena in nanostructures and correlated electron systems

Friday, December 9, 2022 3:30 PM (1h 30m)

The next generation asymmetric horizontal SANS magnet (NHSM) project will provide a unique toolset to study the quantum phenomena in nanostructures and correlated electron systems [1]. This project includes the idea, design and optimization, of a high-performance compensated asymmetric horizontal magnet for small angle neutron scattering (SANS), reflectometry (REFSANS), and the resonance spin echo technique MIEZE (RESEDA) [2]. It uses the new high-temperature superconducting (HTS) technology with a split coil magnet design of reasonable weight (~750kg) and size (~75cm x 75cm), which enables it to fit on several instruments (SANS I, REFSANS, RESEDA, KWS2) at MLZ.

An asymmetric coil geometry removes zero-field nodes and will allow the use of polarized neutrons and polarization analysis. The use of high-temperature superconductor breaches the limitations of stray fields down to 10G at a 1m distance with active compensation at a central field of 10T. This project proposal is based on the results of two feasibility studies performed in collaboration with the companies Bilfinger-Noell (Germany) and HTS-110 (New Zealand), funded by BMBF.
[1] Magnetic Small-Angle Neutron Scattering, S. Mühlbauer et al.,Reviews of Modern Physics, 91, 015004, 2019
[2] Neutron MIEZE spectroscopy with focal length tuning, J. Jochum, A. Wendl, T. Keller and C. Franz. Measurement Science and Technology, Vol. 31, No.3 2020

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Session Classification: Poster Session

Track Classification: Neutron Methods

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

Comparison of pulsed and continuous neutron sources for MIEZE

Friday, December 9, 2022 3:30 PM (1h 30m)

The MIEZE method, a sub-type of the neutron spin echo (NSE) technique, circumvents the coupling of neutron beam phase space and resolution, by using oscillating neutron intensity as an internal clock to record minuscule changes to the energy of a scattered neutron. As a result MIEZE achieves an energy resolution down to the ns range with a bandwidth of $\Delta\lambda/\lambda \approx 10$ %.
This concept has been successfully implemented in the MIEZE spectrometer RESEDA at the reactor source FRM II, studying magnetic dynamics, quantum phenomena and molecular diffusion in soft matter. However, a significant part of the continuously produced neutrons are discarded by the velocity selector, which is why concepts of MIEZE instrumentation at pulsed neutron sources (PNS), which are capable of using the full wavelength spectrum contained in each pulse, are becoming more and more attractive.
We have implemented the polarization shaping components of RESEDA in the McStas framework to investigate the feasibility, data reduction and operation of a MIEZE spectrometer at a PNS. Due to the large wavelength spread of a PNS, the intermediate scattering function can be measured over many points in Fourier time, analogous to a multi-detector option at a triple-axis spectrometer. Simulation of a quasielastic sample allows the comparison of the performance between a continuous neutron source and a PNS, while testing majorly important data reduction algorithms, which have never been addressed in instrument proposals.

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Presenter: FELLNER, Korbinian (TU München)

Session Classification: Poster Session

Track Classification: Neutron Methods

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

Dynamical and structural properties of undercooled Cu-Ti melts

Friday, December 9, 2022 3:30 PM (1h 30m)

Cu-Ti alloys feature a large, undercooled liquid region and a high glass-forming ability (GFA) and thus, provide the possibility to obtain two component bulk metallic glasses (BMGs). Such behavior is unusual and could be due to the special properties of the Cu-Ti system: In the melt, it shows a positive excess volume, whereas it still features a negative enthalpy of mixing.
Even though, the scientific interest in Cu-Ti-based BMGs increased, the relevant atomic mechanisms responsible for such good GFA are still to be explored. Here we discuss the temperature-dependent dynamical and structural properties of Cu-Ti melts, within a compositional range of 24 to 69 at% Ti. To obtain accurate data about viscosity, density, and atomic structure, the Cu-Ti samples have been processed without any container using the electrostatic levitation technique. We found a non-monotonous trend of the viscosity, with the highest values at intermediate Ti contents. Surprisingly, this dynamical trend is not reflected by the macroscopic packing fraction, meaning a high viscosity does not necessarily correlate with a dense packing. However, on the atomic scale, x-ray and neutron diffraction measurements reveal a denser, local packing density and a pronounced chemical short-range order, which is based on attractive interactions between Cu and Ti. These short-range interactions can explain the high viscosity, while the macroscopic packing fraction is rather governed by long-range interactions.

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Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **129** Type: **Talk (20 min + 5 min discussion)**

6Mg(NH2)2:9LiH:12LiBD4 as hydrogen storage material: in-operando phase transformation

Thursday, December 8, 2022 3:25 PM (25 minutes)

Hydrogen storage technologies in low weight hydrides promise to help with the global aim of CO2-emissions reduction. High mass energy densities are needed e.g. for heavy-load long distance mobility like trains, trucks, and airplanes. One of the potential reaction based systems is Mg(NH2)2+LiH with a reversible hydrogen capacity of 5.6 wt.% below 200oC. The kinetics of hydrogen desorption/reabsorption is one of the cornerstones of hydrogen storage materials characteristics. The addition of LiBH4 improves it by forming an intermediate phase. It is speculated that subsequent melting improves the hydrogen diffusion, e.g. in the α-phase Li4(BH4)(NH2)3 or β-phase Li4(BH4)2(NH2)2.

The mixtures described in literature are denoted 6:9:x, 6Mg(NH2)2:9LiH:xLiBD4, where x varies from 0.5 to 12. It has been shown that the increase of x leads to faster reaction kinetics at the cost of loss of mass hydrogen capacity (for 6:9:12 down to 2.3 wt.%).

Neutron diffraction measurements at the diffractometer HRPT at PSI were conducted on the ball milled mixture 6Mg(NH2)2:9LiH:12LiBD4. Measurements were performed at several temperatures (RT, 50, 80, 90oC) in a vanadium container and during heating up to 180oC in a steel container while pumping out the released hydrogen. The phase composition was determined in the as-prepared state and in-situ during heating up to the melting transition. The appearance of new phases was registered after cooling back down to the room temperature.

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Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **130** Type: **Talk (20 min + 5 min discussion)**

Identification of vacancy-related defects in photovoltaic thin films

Variable energy positron annihilation lifetime measurements and related density functional theory calculations of positron lifetimes are presented and discussed for two emerging thin film photovoltaic materials, the binary semiconductor Sb_2Se_3 and the halide perovskite $MAPbI_3$. Measurements on a series of Sb_2Se_3 thin film and single crystal samples are presented. DFT calculations provide evidence for the identification of Sb monovacancy defects and divacancies. Measurements on $MAPbI_3$ samples from three groups supported by DFT calculations provide evidence for the identification of Pb vacancy (B-site) related defects. A comparison between DFT calculated lifetime in MA containing halide perovskites with varying anion type are given and discussed. ‘

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Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **131** Type: **Poster**

KWS-3 very small-angle neutron scattering focusing diffactometer at MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

KWS-3 is a very small angle neutron scattering diffractometer operated by JCNS at Heinz Maier-Leibnitz Zentrum (MLZ) in Garching, Germany. The principle of this instrument is one-to-one imaging of an entrance aperture onto a 2D position sensitive detector by neutron reflection from a double-focusing toroidal mirror. In current state, KWS-3 is covering Q-range between 3·10-5 and 2·10-2 Å-1 and used for the analysis of structures between 30 nm and 20 μm for numerous materials from physics, chemistry, materials science and life science, such as alloys, diluted chemical solutions, hydrogels and membrane systems. Within the last few years we have finalized several big "evolutionary"projects; we have completely re-designed and commissioned the main components of the instrument: selector area, mirror positioning system, main sample station at 10m, beam-stop system; implemented new sample stations at 3.5 and 1.3m, second (very-high resolution) detector, polarization and polarization analysis systems; adapted the instrument to almost any existing/requested sample environment like 6-position Peltier furnace (-25℃ to 140℃), high-temperature furnace (< 1600℃), cryostats/inserts (>20 mK), liquid pressure cell (<5 kBar/10-80℃), CO2/CD4 gas pressure cell (<0.5 kBar/10-80℃), humidity cell/generator (5-95%/10-90℃), magnets (horizontal < 3T, vertical < 2.2T), Bio-logic® multimixer stopped flow (5-80℃), rheometer Anton paar (tangential/radial) etc.

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Session Classification: Poster Session

Track Classification: Soft Matter

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

KWS-X: The new SAXS/WAXS Laboratory Beamline at JCNS-MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

The new customized SAXS/WAXS instrument from XENOCS have be installed in the JCNS X-ray laboratory from the end of 2021. As a young member of our small angle scattering instrument by using x ray as beam, the new instrument is equipped with a high flux metal-jet source and a moveable Eiger 2R4M SAXS detector. With additional 4-axis motorized WAXS detector and Bonse-Hart USAXS the scattering vector q can cover a wide area from 0.0002 to 7 Å-1. Compared to other instruments, it also comprises a large sample environment station that can be used with ambient pressure conditions. A large number of sample environmental accessories make it possible to perform experiments at temperatures from -150oC to 1000oC, under shear, tensile, etc. The instrument is under commissioning and is expected the user operation in Autumn 2022.

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Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **133** Type: **Talk (20 min + 5 min discussion)**

Nested Mirror Optics –Towards a New Generation of Neutron Transport Systems?

Thursday, December 8, 2022 5:35 PM (25 minutes)

The advent of high-brilliance neutron moderators has raised the question how to efficiently extract and transport neutrons from such compact sources while maximizing the brilliance transfer to an instrument. Nested mirror optics (NMO) offer a viable and flexible solution for this task by circumventing the under-illumination associated with long neutron guides. A basic version, consisting of an assembly of short elliptic mirrors, is able to image a well-defined volume of beam phase space from the moderator surface onto a target, e.g., a sample or a virtual source. In contrast to neutron guides, each of the NMO's individual mirrors reflects neutrons only within a narrow range of finite angles. Due to its geometrically well-defined reflection kinematics, one can tailor the divergence and spectrum of the transported beam to the needs of an experiment by design of the NMO. The device thus provides a clean beam without depending on optical elements close to the source or the target, which leads to a number of practical advantages.
Besides a presentation of the concept, we will report on experimental results obtained at the multi-purpose instrument MIRA at FRM2 with an elliptic NMO prototype. We will further present results from recent experiments at the BOA beamline at PSI, which included, among others, the imaging of two-dimensional structures. Supported by McStas simulations, we will highlight various potential applications of NMO for neutron scattering and fundamental physics.

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Presenter: HERB, Christoph (TUM)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **134** Type: **Poster**

Upgrades of the hot diffractometer HEiDi for more efficiency and new challenges

Friday, December 9, 2022 3:30 PM (1h 30m)

HEiDi is one of only two single crystal diffractometers (SCD) using hot unpolarized neutrons worldwide. Many scientific topics on compounds in battery or information technology with light and/or highly absorbing elements profit from comprehensive structure analysis up to high Q as well as experiments using absorbing sample environments like pressure cells. In order to maximize the large versatility of HEiDi a small 2D position sensitive detector (PSD) is currently under construction (BMBF grant 05K19PA2). It will expand its efficiency concerning fast and detailed detection of Bragg and diffuse scattering as well as modulated background.
The large available Q range fits also perfectly to pair distribution function (PDF) analysis as new field of research at MLZ, focusing on short-range order phenomena and complementing existing research on the aforementioned topics. Various groups have recently confirmed its high potential for magnetic studies on powders (mPDF, e.g. [1]) and studies on single crystals (3D-PDF, e.g. [2]). Thus, we propose a large PSD as upgrade covering an angular range > 125°. This offers a Q range above 20 Å^{-1} sufficient for PDF studies on magnetic or structural features. A combination with an also proposed radial collimator will allow for powder studies to very high Q on top. Conceptual details will be shown during the meeting.

[1] Frandsen et al. (2017); Phys. Rev. Mat. 1(7), 074412
[2] T. Weber and A. Simonov; J. Appl. Cryst. 47 (2014), 1146-1152

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Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **135** Type: **Invited talk (30 min + 5 min discussion)**

Determination of the cooperativity length in glass forming liquids and polymers

Thursday, December 8, 2022 1:05 PM (35 minutes)

Although the idea of a 'cooperativity'length scale ξ related to the glass transition is now widespread, there is much less consensus on whether this length scale can be related to thermodynamic fluctuations and, if yes, whether one has to consider temperature fluctuations δT. The crucial experiment to this end has to compare values of ξ from 'thermodynamic'formulae to independent values from structural-dynamics experiments.

In a seminal paper, Ernst Donth proposed to assign a length scale to the AC-calorimetric relaxation time using the spatial resolution of quasielastic neutron scattering. The main problem is to find a range of relaxation times that is accessible by both methods. To achieve this, significant progress in the performance of NSE as well as AC calorimetry was required.

A first experiment of this kind was realised on a glass-forming liquid, propylene glycol (PG). The result was that agreement with the thermodynamic calculations was better if temperature fluctuations were accounted for. Nevertheless, in PG the difference between the two thermodynamic estimates is small. Therefore, a material with a higher 'contrast'between the alternatives was used in a second experiment, poly(ethylmethacrylate) (PEMA). In addition, this experiment benefitted from the upgrade of J-NSE with superconducting coils. The new results show a clear agreement with the thermodynamic calculation involving temperature fluctuations.

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Presenter: ZORN, Reiner (Forschungszentrum Jülich)

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **136** Type: **Talk (20 min + 5 min discussion)**

Novel CDB Data Processing and Evaluation Software

Thursday, December 8, 2022 3:00 PM (25 minutes)

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) is currently under development. The software can already 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. This combined with a new multi detector CDB function, which enables the combination of the data from all 10 detectors, provides detailed information about the chemical environment of the positron annihilation site. The software capabilities were tested on W and Kapton measurements with high statistics to investigate materials with both predominantly high and low Doppler shifts. Measurements on the precipitation hardening properties of Al alloy samples were subsequently performed and will be shown.

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Presenter: CHRYSSOS, Leon

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **137** Type: **Talk (20 min + 5 min discussion)**

Fundamentals of diffraction-based residual stress and texture analysis of laser powder bed fused Inconel 718

Thursday, December 8, 2022 5:35 PM (25 minutes)

Laser powder bed fusion (PBF-LB/M) of metallic alloys is a layer wise additive manufacturing process which provides significant scope for more efficient designs of components, benefiting performance and weight, leading to efficiency improvements for various sectors of industry. However, to benefit from these design freedoms, knowledge of the high produced induced residual stress and mechanical property anisotropy associated with the unique microstructures is critical. X-ray and neutron diffraction are considered the benchmark for non-destructive characterization of surface and bulk internal residual stress. The latter, characterized by the high penetration power in most engineering alloys, allows for the use of diffraction angle close to 90° enabling a near cubic sampling volume to be specified. However, the complex microstructures of columnar growth with inherent crystallographic texture typically produced during PBF-LB/M of metallics present significant challenges to the assumptions typically required for time efficient determination of residual stress. These challenges include the selection of an appropriate set of diffraction elastic constants and a representative strain-free reference for the material of interest. In this presentation advancements in the field of diffraction-based residual stress analysis of L-PBF Inconel 718 will be presented. The choice of an appropriate set of diffraction-elastic constants depending on the underlying microstructure will be described.

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Presenter: SCHRÖDER, Jakob

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **138** Type: **Poster**

The GNeuS project - The Call N. 2 offers 15 post-doc positions at the MLZ

Friday, December 9, 2022 3:30 PM (1h 30m)

Research with neutrons, with its interdisciplinary approach, is indispensable for modern science. Taking into consideration tremendous changes in the European neutron landscape and assuming responsibility for sustainability, the neutron community is nowadays facing an important task to ensure long-term perspectives, that essentially depend on its ability to create a new generation of innovative highly-skilled researchers. To tackle this challenge, Forschungszentrum Jülich (FZJ), Technical University Munich (TUM) and Helmholtz-Zentrum Hereon (Hereon), partners at the Heinz-Maier-Leibnitz Zentrum (MLZ), are running the Marie-Skłodowska Curie Acton (MSCA) COFUND project "Global Neutron Scientists"(GNeuS) https://GNeuS.eu that trains young neutron scientists through the establishment of a well-structured post-doctoral research programme with a strong interdisciplinary and intersectoral approach and global outreach. Within GNeuS, Post-Doc grants are offered to solving the grand challenges facing mankind in areas such as environment, energy, key technologies and life science as well as improving the existing instrumentation and the ancillary equipments and developing new sources or optimizing the existing ones.

The GNeuS Call N. 2 opens on November 1, 2022, and the application submission deadline is on January 18, 2023, at 18:00 CET. The candidate is warmly invited to submit the application by completing the application package via the GNeuS Portal https://my.gneus.eu.

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Presenter: CARSUGHI, Flavio (Forschungszentrum Juelich)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **139** Type: **Talk (20 min + 5 min discussion)**

Optimized signal deduction procedure for the MIEZE spectroscopy technique

Thursday, December 8, 2022 5:10 PM (25 minutes)

A method is reported to determine the phase and amplitude of sinusoidally modulated event rates, binned into four bins per oscillation, based on data generated at the resonant neutron spin-echo spectrometer RESEDA at FRM-II. The presented algorithm relies on a reconstruction of the unknown parameters. It omits a calculation-intensive fitting procedure and avoids contrast reduction due to averaging effects. It allows the current data acquisition bottleneck at RESEDA to be relaxed by a factor of four and thus increases the potential time resolution of the detector by the same factor. The approach will be compared with the established fitting procedures of time series having four and 16 time bins per oscillation. In addition the empirical estimates of the errors of the three methods are presented and compared with each other. The reconstruction is shown to be unbiased, asymptotic and efficient for estimating the phase. Reconstructing the contrast increases the error bars by roughly 10% as compared with fitting 16 time-binned oscillations. Finally, we present heuristic, analytical equations to estimate the error for phase and contrast as a function of their initial values and counting statistics.

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Presenter: SOLTWEDEL, Olaf

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **140** Type: **Poster**

Mechanism of Na+ diffusion in NASICON solid electrolyte materials studied by Quasi-Elastic Neutron Scattering

Friday, December 9, 2022 3:30 PM (1h 30m)

The sodium superionic conductor materials, also known as NASICON, 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 clarify the reason for extremely high conductivity exhibited by some compositions, specifically by Na1+xZr2SixP3-xO12 ($0 \leq x \leq 3$), and to explain the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at around 170℃, on the Na+-ion occupancy. We also investigate the role of Al/Y and Sc substitution and the overall temperature dependence of the ionic conductivity in the temperature range of 297-640K.

The quasi-elastic neutron scattering (QENS) is used to measure the spatial and temporal dynamic properties of diffusion of Na+ ions in the crystal structure. The measurements were performed at the BASIS spectrometer at the SNS, Oak Ridge National Laboratory in Tennessee, USA.

The Na+ ion diffusion mechanism can be described by the right choice of the diffusion model, Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data. Additionally, temperature dependent X-ray diffraction data have been obtained and analysed. Information about interatomic distances have been extracted in order to confirm the results obtained from the QENS data.

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Presenter: PIVARNÍKOVÁ, Ivana

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **141** Type: **Poster**

Influence of build direction on residual stresses and textures in lightweight alloys produced by additive manufacturing (AM).

Friday, December 9, 2022 3:30 PM (1h 30m)

The freedom in complexity of AM metal parts allows very stiff and extreme light designs made of AlSi11Mg0.5 alloy and are entering serial production in automotive industry amongst others. Nevertheless, the production process of laser powder bed fusion (LPBF) is prone to the formation of residual stresses (RS). Furthermore, the parts may have distortions and must undergo a subsequent heat treatment to release RS, which is cost and energy intensive or not possible at all. Therefore, a pro-found understanding of the formed RS is mandatory for structural integrity assessment and successful industrial manufacturing suitable for industry. The LPBF production process is closely linked to texture formation, which results in anisotropic mechanical properties.
In the current presentation, we investigate the evolution of residual strains and texture of an additively manufactured AlSi11Mg0.5 alloy component as function of building directions. This preliminary study uses high energy synchrotron X-rays to assess the strains of the different phases in this alloy and corresponding pole figures are derived to correlate the texture with the resulting stress profiles. In addition the influence of heat treatment on the strain level is studied as a function of spatial position within the AM parts. A brief outlook how this results can be used and further extended by neutron diffraction measurements to qualify and mitigate stress induced failure mechanisms in real parts will also be given.

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Presenter: WALZ, Erik (FRM II / STRESS-SPEC)

Session Classification: Poster Session

Track Classification: Material Science

Contribution ID: **142** Type: **Poster**

vBambus: a multiplexing backend for the Panda virtual Instrument

Friday, December 9, 2022 3:30 PM (1h 30m)

At the cold triple axis instrument PANDA, a virtual twin based on Monte-Carlo ray-tracing simulations is used for educational purposes in student practical, training of newly arrived staff and experiment planning for users. The underlying McStas simulation is connected to the NICOS instrument control software, giving the virtual twin the look and feel of the real instrument. Also, instrumental properties like the resolution are accurately reproduced. Furthermore, at PANDA the multiplexing backend BAMBUS is waiting for its first neutrons. Here we report the implementation of BAMBUS with its 100 analysers and detectors into the virtual twin experiment. For this purposes, the McStas instrument file is created using a python script. The compiled virtual instrument is then connected to Nicos. Using a simple virtual sample, the data reduction using the Mjolnir software package can already be tested without neutrons.

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Co-authors: SCHNEIDEWIND, Astrid; FRANZ, Christian

Presenters: LÖSCH, Augustin; Mr BAUER, Lukas (Jülich Forschungszentrum GmbH)

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **143** Type: **Poster**

Small-angle neutron scattering of kinetically driven skyrmion lattice motion

Friday, December 9, 2022 3:30 PM (1h 30m)

Skyrmions are topologically non-trivial spin textures that exhibit an exceptionally efficient coupling to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe, and Cu2OSeO3 [1, 2, 3]. This raises the question for the microscopic mechanisms that control the pinning of the skyrmion lattice, and how they depend on the topology, electronic structure, and disorder.

We report neutron scattering measurements of kinetically driven skyrmion lattice unpinning and motion by means of Time-Involved Small Angle Neutron scattering Experiment (TISANE) [4]. By interlocking the phases of neutron pulse, sample modulation, and detector signal, the technique allows to record data without major sacrifice in intensity at time-scales down to micro-seconds and provides a direct insight on the skyrmion lattice motion.

In our study we examined the unpinning process under changing field orientation for different materials including the metallic systems Mn1–xFexSi and the insulator Cu2OSeO3. We discuss our results in the light of methodological aspects of the TISANE technique and recent theoretical predictions of walking skyrmions.

[1] T. Schulz et al., Nat. Phys. 8, 301-304 (2012).
[2] K. Everschor et al., PRB 86, 054432 (2012).
[3] S. Zang et al., Nat. Comm. 9, 2115 (2018).
[4] S. Mühlbauer et al., New J. Phys. 18, 075017 (2016).

Primary authors: METTUS, Denis (Technische Universität München); CHACON, Alfonso; BAUER, Andreas (Technische Universität München); MUEHLBAUER, Sebastian; BEZVERSHENKO, Alla (Institute for Theoretical Physics, University of Cologne); HEINEN, Lukas (Institute for Theoretical Physics, University of Cologne); Prof. ROSCH, Achim (Institute for Theoretical Physics, University of Cologne); PFLEIDERER, Christian

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Session Classification: Poster Session

Track Classification: Quantum Phenomena

Contribution ID: **144** Type: **Invited talk (30 min + 5 min discussion)**

The 10B based JALOUSIE neutron detector: its current status and its employment for POWTEX at FRM II as well as DREAM and MAGiC at ESS

Thursday, December 8, 2022 1:05 PM (35 minutes)

JALOUSIE is a modularized neutron detector concept that has been realized for the first time in POWTEX. It was developed to serve as alternative for classical 3He position sensitive detector tubes as used for large neutron scattering instruments. POWTEX has been fully instrumented at FRM II along this concept. Further JALOUSIE based systems are under production for DREAM and MAGiC at ESS.
The comparatively small overall detection efficiency of an individual 10B4C layer is enhanced by tilting with 10° the layer towards the incoming neutron path, thus increasing the effective absorption depth by a factor of 6. Additionally, 8-12 such conversion layers are arranged along any neutron path to further enhance overall detection efficiency to 54%-63% at 1 Å. Consequently, JALOUSIE provides a 3-dimensional detection volume structured into highly granular voxels for readout. Spatial resolution of 5-7 mm (FWHM) and down to 1 mm (FWHM) in a special configuration along one dimension as well as time of flight resolution of 3-10 µs (FWHM) may be customized through design parameters.
The detector concept will be presented together with test measurement results, which document the seamlees operation of the detector system. Further variants of the concept as implemented at DREAM and MAGiC will be indicated.

Primary author: KLEIN, Martin (CDT CASCADE Detector Technologies GmbH)

Presenter: KLEIN, Martin (CDT CASCADE Detector Technologies GmbH)

Session Classification: Neutron Methods

Track Classification: Neutron Methods

Contribution ID: **145** Type: **Poster**

GISANS at high pressure

Friday, December 9, 2022 3:30 PM (1h 30m)

The investigation of thin films with Grazing Incidence Small Angle Neutron Scattering (GISANS) has been established as an advanced characterization method in the last years. Lateral structures from the nanometer to the micrometer range are accessible and different sample environments were developed for GISANS experiments under controlled environmental conditions. However, so far the access to high pressure GISANS was very limited. Therefore, we present recent and ongoing developments at MLZ for GISANS experiments under high pressure. This is a joint collaboration between MLZ and ILL. Based on an existing pressure cell [1] that had originally been used for neutron reflectometry experiments and was used successfully elsewhere, we develop a novel pressure cell for GISANS to be used primarily at MLZ. The pressure cell enables a pressure range between 1 bar to at least 1000 bar, which is highly relevant for thin films in the soft matter area. Particular emphasis is placed in the optimization of the sample volume and cell windows for a robust and versatile operation in GISANS mode to probe thin polymer films. GISANS tests are going to be launched at SANS-1 beamline.

[1] Martin Kreuzer, Thomas Kaltofen, Roland Steitz, Beat H. Zehnder, and Reiner Dahint, "Pressure cell for investigations of solid–liquid interfaces by neutron reflectivity", Review of Scientific Instruments 82, 023902 (2011)

Primary authors: Dr VAGIAS, Apostolos (FRM2 / TUM); BUCHNER, Andreas; SCHULTE, Alfons (University of Central Florida); GUTFREUND, Philipp (ILL); MUEHLBAUER, Sebastian; WILHELM, Andreas; MÜLLER-BUSCHBAUM, Peter (Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany; MLZ, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany)

Presenter: Dr VAGIAS, Apostolos (FRM2 / TUM)

Session Classification: Poster Session

Track Classification: Soft Matter

Contribution ID: **146** Type: **Poster**

Integration of eWorkbench into NICOS

Friday, December 9, 2022 3:30 PM (1h 30m)

NICOS is a network-based control system written for neutron scattering instruments, originally at the MLZ. Its main goals are flexibility, ease of use and maintenance, and reusability. NICOS allows remote control of scientific instruments via both interactive interfaces (GUI, command line) and a scripting system.

eWorkbench is a generic platform for managing research data and projects. It facilitates data management by enabling collaboration and semi-automatic documentation. Among other things eWorkbench offers convenient integration of labbooks with the possibility of creating notes, comments, sketches, uploading files, pictures and structuring with different sections.

Here we use the eWorkbench API to transfer the output from NICOS's electronic labbook to a labbook from eWorkbench. Sophisticated user authorization will be deployed to fully meet the requirements of making the web-based eWorkbench application safe and user-friendly at the same time.

Primary author: BAUDISCH, Josef

Presenter: BAUDISCH, Josef

Session Classification: Poster Session

Track Classification: Neutron Methods

Contribution ID: **147** Type: **Talk (20 min + 5 min discussion)**

Substructure decoration with gamma radiation of rock salt (NaCl) for transmitted light optical microscopy - a review

Thursday, December 8, 2022 4:15 PM (25 minutes)

Inspired by the possible storage of nuclear waste in impermeable rock salt formations, numerous theoretical and applied studies have investigated the effect of gamma irradiation on the structural properties of halite over the last five decades. An important discovery has been the gamma irradiation - induced decoration of othervise invisible lattice defect substructures in this optically isotropic mineral (Urai et al, 1986; Donker and Garcia Celma, 1996). This is used to unravel the geologic history of the rock salt. The decoration of defects is caused by the heterogeneous nucleation of colloidal Na at specific conditions of irradiation dose rate, temperature, and total dose (Opbroek and Hartog, 1984). However, although the development of total stored energy is well known as a function of these parameters, the distribution of the colloidal Na as a function of defect structure is not well understood and provides an opportunity to further develop the method. In this review, we present examples of microstructural studies of thin sections in the optical microscope and outline the path towards optimalization and standardization of the method. Currently, defect decoration in natural rock salt is being further investigated using the FRM II gamma irradiation facility (Li et al, 2022).

Urai et al., 1986. https://doi.org/10.1038/324554a0
Donker and Garcia Celma, 1996. https://doi.org/10.108/10420159608212929

Primary author: Dr SCHMATZ, Joyce (MaP - Microstructure and Pores GmbH)

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Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **148** Type: **Talk (20 min + 5 min discussion)**

Molecular Understanding of the Dynamics of Supramolecular Polymers across different Length Scales

Thursday, December 8, 2022 2:05 PM (25 minutes)

Supramolecular polymers offer exciting prospects for materials with novel properties because of the reversibility of the non-covalent interactions, like H-bonding.[1,2] This work aims to unravel the correlation between H-bonding association and main chain polarity in supramolecular polymer melts. These are based on poly(ethylene)oxide (PEO) and poly(propylene)oxide (PPO) (in order of decreasing polarity) polymers possessing at the ends either the pair diaminotriazine (DAT) and thymine-1-acetic acid (THY) or 2-ureido-4[1H]-pyrimidinone (UPY) as H-bonding functional groups. A combination of rheology, DRS and NSE provided the association lifetimes for the supramolecular PEO and PPO functionalized with the pair THY/DAT.2 The lifetimes for THY/DAT are the same for supramolecular PEO and PPO and independent of the chain polarity. SANS results reveal that while PEO and PPO functionalized with THY/DAT self-assemble as linear chains, PEO and PPO functionalized with UPY show phase separation with a cluster size of ~3 nm responsible for the physical crosslinks of the formed transient network.[2,3]

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1 A.Brás, A.Arizaga, D.Sokolova, U.Agirre, S.Prévost, A.Radulescu, M.T.Viciosa, M.Kruteva, W.Pyckhout-Hintzen, A.M.Schmidt, Macromolecules, submitted.
2 A.Brás, A.Arizaga, U.Agirre, M.Dorau, J.Houston, A.Radulescu, M.Kruteva, W.Pyckhout-Hintzen, A.M.Schmidt, Polymers, 2021,13, 2235.

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Presenter: BRÁS WÜRSCHIG, Ana (University of Cologne (UzK))

Session Classification: Soft Matter

Track Classification: Soft Matter

Contribution ID: **149** Type: **Talk (20 min + 5 min discussion)**

Design and construction of a levitated dipole trap for pair plasma studies

Thursday, December 8, 2022 4:15 PM (25 minutes)

Magnetic dipole traps have demonstrated good confinement properties for both non-neutral and quasi-neutral plasmas, making them highly suitable for the creation and study of low-temperature, long-lived electron-positron pair plasmas. To generate such a plasma, the APEX (A Positron-Electron eXperiment) Collaboration is planning to inject positrons (supplied by the reactor-based beam NEPOMUC, then collected into pulses in a buffer-gas trap) into a dipole magnetic field, which is previously loaded with a comparable population of electrons. Our dipole trap is a 15-cm-diameter high-temperature superconducting (HTS) closed coil, which is cryogenically cooled (20 K) and inductively charged (56 kAt, B_{axis}= 0.5 T). Levitation prevents particle losses through the intersection of magnetic field lines with material surfaces (e.g. mechanical supports). By directly exposing the coil to room temperature thermal radiation, we observed a worst-case warming rate that limits available levitation time to 96 min. Simulations have shown that a technique for injecting positrons across magnetic field lines (previously demonstrated in a prototype supported dipole trap) is expected to be transferrable to the higher fields and symmetric geometry of the levitated dipole trap. The construction of the levitated dipole trap itself is nearing completion, with commissioning and electron experiments anticipated to take place by the end of 2022.

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Presenter: CARD, Alexander (Max-Planck-Institut für Plasmaphysik)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **150** Type: **Poster**

Design considerations of UV-visible Microspectroscopy at single crystal neutron diffractometers

Friday, December 9, 2022 3:30 PM (1h 30m)

Single crystal neutron diffraction experiments on protein crystals often require beamtimes of several days in order to measure a complete data set which leads to meaningful results on atom positions and occupancies. In case of room temperature measurements, the sample under investigation might change during that time. If one wants to study a radical intermediate state of the protein, often linked to a distinct UV-visible absorption of the crystal, one is often interested in the decay of the number of radicals in the crystal. Below a certain number, one would rather switch to another freshly prepared crystal. This would save precious neutron beamtime.
At synchrotron beamlines, UV-Visible microspectroscopy of the crystals mounted on the goniometer is readily available. The purpose of this set-up is to measure the UV-visible spectrum on an oriented crystal on the beamline without the need to take it off the beamline goniometer. This has the advantage that the crystal orientation relative to the light beam and polarization is known. Furthermore, a crystal unmounting step can be avoided for just measuring its UV-visible spectrum.
At neutron instruments, such microspectroscopy set-ups are usually not found. But this set-up could also be used to detect whether a ligand is present in a crystal, when the ligand has some optical absorption fingerprint. In this contribution I will discuss some design considerations of such a set-up.

Primary author: SCHRADER, Tobias

Presenter: SCHRADER, Tobias

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **151** Type: **Talk (20 min + 5 min discussion)**

Moving into higher fields and collective behavior: recent advancements toward matter-antimatter pair plasmas

Thursday, December 8, 2022 3:50 PM (25 minutes)

The ultimate goals of the APEX (A Positron Electron eXperiment) Collaboration are the generation and investigation of con□ned, strongly magnetized, electron-positron plasmas in the laboratory. The mass symmetry of such plasmas simplifies many aspects of their physics, as has been described in more than four decades of theory/simulation predictions.

Our road map to conducting experimental studies requires unifying and advancing state-of-the-art physics and engineering in several areas, including:
• extended accumulation and high-capacity storage of large numbers of positrons (originating from NEPOMUC);
• two superconducting, tabletop-sized toroidal con□nement devices with complementary magnetic topologies (a dipole and a stellarator), in which the positrons will be combined with electrons and their plasma properties studied; and
• the development and verification of a number of essential enabling techniques — e.g., efficient transport of positrons across magnetic □ux surfaces and subsequent trapping (previously demonstrated in the single-particle regime).

This talk will provide a broad overview of recent headway made along that road map, which has included progress in non-neutral plasma trapping; the further development of the positron beam and techniques for injecting it into toroidal geometries, including with an electron space charge present; and the development of the toroidal traps.

Primary authors: STENSON, E. V. (MPI für Plasmaphysik); CARD, A. (MPI für Plasmaphysik); DANIELSON, J. R. (UC San Diego); DELLER, A. (MPI für Plasmaphysik); HERGENHAHN, U. (Fritz-Haber-Institut der MPG); HORN-STANJA, J. (MPI für Plasmaphysik); HUGENSCHMIDT, C. P. (TUM); HUSLAGE, P. (MPI für Plasmaphysik); VON DER LINDEN, J. (MPI für Plasmaphysik); NISSL, S. (MPI für Plasmaphysik); PEDERSEN, T. Sunn (MPI für Plasmaphysik); ROGGE, C. W. (TUM); SAITOH, H. (University of Tokyo); SCHWEIKHARD, L. (University of Greifswald); SINGER, M. (MPI für Plasmaphysik); SINGER, M. (MPI für Plasmaphysik); SMONIEWSKI, J. (MPI für Plasmaphysik); STEINBRUNNER, P. (MPI für Plasmaphysik); SURKO, C. M. (UC San Diego); STONEKING, M. R. (Lawrence University)

Presenter: STENSON, E. V. (MPI für Plasmaphysik)

Session Classification: Positrons

Track Classification: Positrons

Contribution ID: **152** Type: **Invited talk (30 min + 5 min discussion)**

Neutron imaging in materials science

Thursday, December 8, 2022 1:05 PM (35 minutes)

Imaging techniques based on neutron beams are rapidly developing and have become versatile non-destructive analysing tools in many research fields. Due to their intrinsic properties, neutrons differ strongly from electrons, protons or X-rays in terms of their interaction with matter: they penetrate deeply into most common metallic materials while they have a high sensitivity to light elements such as hydrogen, hydrogenous substances or lithium. This makes neutrons perfectly suited probes for research on materials that are used for energy storage and conversion, e.g. batteries, hydrogen storage, fuel cells, etc. Moreover, their wave properties can be exploited to perform diffraction, phase-contrast and dark-field imaging experiments. Their magnetic moment allows for resolving magnetic properties in bulk samples. This presentation will focus on recent applications of neutron imaging techniques in both materials research and fundamental science illustrated by examples selected from different areas.

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Presenter: KARDJILOV, Nikolay (Helmholtz-Zentrum Berlin)

Session Classification: Material Science

Track Classification: Material Science

Contribution ID: **153** Type: **Talk (20 min + 5 min discussion)**

Revealing the origin of additional voltage steps of over-lithiated high voltage spinel

Thursday, December 8, 2022 4:15 PM (25 minutes)

High voltage spinel LiNi0.5Mn1.5O4 is considered as one of the most promising cathode material for next generation lithium ion batteries. The material is expected to be significantly cheaper and more safe than state of the art layered oxides, while providing high specific energy of 690 Wh/kg. Yet this material possesses another highly interesting feature which is the possibility of over lithiation up to x=2.5 in LixNi0.5Mn1.5O4. Utilizing the full compositional range 0<x<2.5, nickel manganese spinel theoretically provides up to 1190 Wh/kg. However, cycling the material to full extend leads to pronounced capacity fading. The reason for this aging is not yet understood and so are the additional voltage step at 2.1 observed during lithiation and the linear voltage slope from 2.0 to 1.5 V, and the additional voltage step at 3.8 V observed during de-lithiation. Only by applying several complementary characterisation methods as operando XRD, neutron diffraction and potentiostatic entropymetry, we were able to attribute the voltage steps to a tetragonal phase of the spinel with lithium ions on octahedral and tetrahedral sites and a metastable cubic phase with lithium ions also located on both octahedral and tetrahedral sites. Therefore this work provides the basis for further material design.

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Presenter: JOBST, Nicola (ZSW)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **154** Type: **Poster**

High-throughput powder diffractometer ERWIN – design, capabilities and opportunities

Friday, December 9, 2022 3:30 PM (1h 30m)

Powder diffraction at neutron sources stands in the forefront of materials research and powder diffractometers are standard working horses at large scale facilities serving a large part of neutron community with data and producing the vast of scientific output. Many years ago the analysis of instrumental suite at FRM II reactor source clearly identified a demand for high-throughput monochromatic diffraction instrument, addressing a large section of reciprocal space in gapless fashion and adopting sufficient dynamic range with μs time-resolution, suited for both rapid data collection and studies of small sample volumes in the range of mm3, allowing for a variety of different sample environments and having a capability to eliminate their contributions.
In the current contribution a final concept of medium-resolution neutron powder diffraction option ERWIN at beam port SR8b at FRM II will presented. By its design the instrument ERWIN –"Energy research with neutrons"is especially adapted for structural characterization of energy materials and electrochemical storage systems by applying simultaneous bulk/spatially resolved neutron powder diffraction. Besides this a number of useful experimental options and features enabling studies of small samples using an adapted radial collimator, rapid parametric measurements as a function of external parameters, time-resolved studies etc will be discussed.

Primary author: SENYSHYN, Anatoliy

Presenter: SENYSHYN, Anatoliy

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **155** Type: **Talk (20 min + 5 min discussion)**

Magnetic properties of the noncentrosymmetric tetragonal antiferromagnet $EuPtSi_3$

Thursday, December 8, 2022 2:05 PM (25 minutes)

We report a comprehensive study of single crystals of the noncentrosymmetric rare-earth compound $EuPtSi_3$ grown by the optical floating-zone technique. Measurements of the magnetization, ac susceptibility, and specific heat consistently establish antiferromagnetic order of localized Eu^{2+} moments below the Néel temperature $T_N = 17$ K, followed by a second magnetic transition at $T_{N1} = 16$ K. For a magnetic field along the easy $[001]$ axis, the magnetic phase diagram is composed of these two phases. For fields applied in the magnetically hard basal plane, two additional phases emerge under magnetic field, where the in-plane anisotropy is weak with $[100]$ being the hardest axis. At the phase transitions, the magnetic properties exhibit hysteresis and discrepancies between differential and ac susceptibility, suggesting slow reorientation processes of mesoscale magnetic textures. Consistently, powder and single-crystal neutron diffraction in zero field identify magnetic textures that are modulated on a length scale of the order of 10 nm. Using a full linear polarization analysis of resonant elastic x-ray scattering data, we identify the four long-range ordered phases as variations of noncollinear antiferromagnetic order.

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Co-authors: Dr AQEEL, Aisha (Technische Universität München); SENYSHYN, Anatoliy; Prof. BACK, Christian (Technische Universität München); FRANZ, Christian; Dr SEARS, Jennifer (DESY); Dr MEVEN, Martin (RWTH Aachen University, Institute of Crystallography - Outstation at MLZ); Dr BERECIARTUA PEREZ, Pablo (DESY); Mrs BOZHANOVA, Ralitsa (Technische Universität München); Dr GOTTLIEB-SCHÖNMEYER, Saskia (Technische Universität München); Dr FRANCOUAL, Sonia (DESY); SCHRADER, Tobias

Presenter: BAUER, Andreas (Technische Universität München)

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **156** Type: **Poster**

High-Resolution Powder Diffractometer SPODI – Status and Perspectives

Friday, December 9, 2022 2:00 PM (3 hours)

In this presentation, we will give an overview of the current status of the powder diffractometer SPODI 1, its performance in user service together with future perspectives. In this respect, the impact of the foreseen new SR8 shielding and neutron optics setup on instrumental resolution and flux characteristics will be addressed as well as current developments in sample environment. In addition, an overview on the research areas and outcome in user service will be provided.

References:
1 Nuclear Instruments and Methods in Physics Research A 667 (2012) 32–37.

Primary author: HOELZEL, Markus

Co-authors: SENYSHYN, Anatoliy; HAUF, Christoph; Dr STRANGMÜLLER, Stefan (Technische Universität München - Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II)); PFANZELT, Josef (MLZ); EHRENBERG, Helmut (KIT)

Presenter: HOELZEL, Markus

Session Classification: Poster Session

Track Classification: Structure Research

Contribution ID: **157** Type: **Invited talk (30 min + 5 min discussion)**

Challenges and opportunities in UCN science: new sources and novel detectors

Thursday, December 8, 2022 1:05 PM (35 minutes)

In-situ experiments with ultracold neutrons (UCN) present an opportunity to profit from long observation times and high densities, but must confront numerous practical challenges. I will discuss the challenges and opportunities connected with *in-situ* measurements of the neutron's electric dipole moment, focusing on a modular multichamber concept based on UCN production, storage, and detection in small cells filled with isotopically pure superfluid helium. Key challenges include in-situ UCN detection with spin selectivity, and the management of systematic errors arising from nondynamical phase shifts. I will discuss possibilities for UCN detection and readout, as well as concepts for implementing them in demonstration- and full-scale experiments. Requirements for magnetic shielding and magnetometry will also be surveyed.

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Presenter: DEGENKOLB, Skyler (Universität Heidelberg)

Session Classification: Nuclear, Particle and Astrophysics

Track Classification: Nuclear, Particle and Astrophysics

Contribution ID: **158** Type: **Talk (20 min + 5 min discussion)**

The half- to full-Heusler transition in Ni_{1+x}MnSb

Thursday, December 8, 2022 1:40 PM (25 minutes)

Structural voids are a defining feature of the half-Heusler structure. Using temperature-dependent neutron diffraction, the disordering of these vacancies is followed across the $C1_b$-$L2_1$ transition in samples of $Ni_{1+x}MnSb$ for various Ni excesses x, demonstrating the second-order nature of this transition. Structure solution on high-resolution room-temperature neutron diffraction as well as X-ray diffraction data yields a vacancy content in excess of $1 - x$, the concentration of constitutional vacancies in the ideal model of site occupations. This is mirrored by the increased lattice constant during temperature-dependent diffraction on cooling, implying an annihilation of the initial vacancy excess at elevated temperatures. The reason for this very slow time-scale of vacancy concentration equilibration as compared to typical systems will be discussed, and consequences for the materials properties will be pointed out.

P. Neibecker et al., *phys. status solidi B* **259**, 2100174 (2022)

Primary author: LEITNER, Michael

Co-author: NEIBECKER, Pascal

Presenter: LEITNER, Michael

Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **159** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Nuclear, Particle and Astrophysics

Contribution ID: **160** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Soft Matter

Contribution ID: **161** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Material Science

Contribution ID: **162** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Neutron Methods

Contribution ID: **163** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Quantum Phenomena

Contribution ID: **164** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Positrons

Contribution ID: **165** Type: **not specified**

Welcome

Thursday, December 8, 2022 1:00 PM (5 minutes)

Session Classification: Structure Research

Contribution ID: **166** Type: **Invited talk (30 min + 5 min discussion)**

Neutron diffraction competing with high resolution X-ray diffraction: Any chances?

Thursday, December 8, 2022 1:05 PM (35 minutes)

Structural investigations on functional ceramics is an important tool for material characterisation and tailoring of properties for specialised applications. This frequently requires high angular resolu-tion to resolve highly correlated phase coexistences or subtle structural features. The most common tool is high resolution X-ray or synchrotron radiation. Especially for in situ investigations in transmission geometry, synchrotron facilities are the usual choice. In special cases even optimised setups with 2D detectors are not able to resolve weak reflection splitting of phase coexistences. Then analyser detectors with a resolution at the physical limit are necessary. However, with increasing brilliance and decreasing beam sizes at the synchrotron sources, the grain statistics become a significant challenge and in some cases the feasible experiments are limited to microstructures with grain sizes in the low µm range.
Since many material systems exhibit grain sizes well above this limit, other characterisation methods are necessary. Here the unique properties of neutron instruments can be exploited. Due to the usually rather high wavelengths, the minimum in the curve of reflection widths lies at relatively high angles. Together with the high reflection intensities at high diffraction angles, these setups can be a real competitor for synchrotron instruments. We will demonstrate this with two examples in the material systems potassium sodium niobate and barium titanate.

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Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **167** Type: **Talk (20 min + 5 min discussion)**

Neutron depolarization measurements on HgCr2Se4 under pressure

Thursday, December 8, 2022 2:05 PM (25 minutes)

The pressure dependent magnetic phase diagram of chromium spinel $HgCr_2Se_4$ was investigated up to 6 GPa. Hydrostatic pressure was applied with purposely built diamond anvil cells. The magnetic state of the samples was probed by neutron depolarization, where a pair of focusing neutron supermirror guides was used, increasing the signal intensity by a factor 20. The use of the neutron guides allowed forn an increase of an order of magnitude in the signal to noise ratio while maintaining the exposure time, compensating for the very small sample size insdie the diamond anvil cell. Given the strong competition between FM and AFM exchange in $HgCr_2Se_4$ and parent compounds, the different ground states and physical phenomenon observed are likely a consequence of complex coupling of structural distortions with the magnetic degrees of freedom.

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Session Classification: Quantum Phenomena

Track Classification: Quantum Phenomena

Contribution ID: **168** Type: **Talk (20 min + 5 min discussion)**

Exchange interactions and phase transitions in an external magnetic field in orthoferrites RFeO3 (R=Ho,Tb,Yb).

Thursday, December 8, 2022 3:00 PM (25 minutes)

Rare-earth orthoferrites RFeO3 represent an interesting and importantnfamily of magneticncompounds. Their remarkable magnetic properties result from complex interactions between the moments of the 3d electrons on the transition metal and the 4f electrons on the rare-earth atoms.These interactions lead to the presence of magnetoelectric properties and to the magnetocaloric effect in compounds RFeO3. Its compounds crystallize in structure with the space group Pnma. At the Neel temperature which is typically in the range TN = 600 ÷ 700 K, the iron magnetic moments form a canted antiferromagnetic phase, where the Dzyaloshinsky-Moriya interaction is responsible for the canting of the Fe-sublattice.
We have performed studies of the TbFeO3 by triple-axis neutron spectroscopy on the PUMA (MLZ). The obtained exchange parameters between nearest neighbors for Fe3+ in TbFeO3 have different values for the exchange within the ac plane and along the b-axis: 4.55(2) meV against 4.77(1) meV. This result compares with our previous measurements of HoFeO3 1 and data from literature for YbFeO3 2. Such approach allow us to describe spin reorientation transitions in an external magnetic field in terms of the energy balance of the system. This in good agreement with our experiments on neutron diffraction, which were performed on instruments POLI (MLZ) and D23 (ILL).

1 A.K. Ovsyanikov, et al., JMMM 507 (2020)
2 S. E. Nikitin, et al., Phys. Rev. B 98, (2018)

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Session Classification: Structure Research

Track Classification: Structure Research

Contribution ID: **169** Type: **Plenary talk**

Total-scattering methods as a probe of local structure and correlated disorder in materials

Friday, December 9, 2022 9:00 AM (45 minutes)

The structures of materials under study are of ever-increasing complexity, now often exhibiting short-range order, nano-structure, or correlated disorder that affect their physical and/or functional properties. In order to quantify this increasing structural complexity, a maximal amount of information needs to be extracted from e.g. neutron diffraction patterns, whence the importance of total-scattering techniques accompanied by Fourier methods such as Pair-Distribution Function analysis. Proper interpretation of the experimental results requires an understanding of the space and time scales of the material's structure, as compared to those of the structural measurement.

Primary author: FISCHER, Henry E. (ILL)

Presenter: FISCHER, Henry E. (ILL)

Session Classification: Plenary

Contribution ID: **170** Type: **Plenary talk**

German Committee Research with Neutrons (KFN)

Presenter: BRADEN, Markus (Universität zu Köln)

Session Classification: Plenary

Contribution ID: **171** Type: **Plenary talk**

Phonons at Electronic Phase Transitions

Friday, December 9, 2022 9:45 AM (45 minutes)

Lattice vibrations, i.e., phonons are ubiquitous in solids and getting detailed knowledge on them was one of the success stories of early inelastic neutron scattering. Nowadays, large neutron detectors along with *ab-initio* lattice dynamical calculations allow comprehensive experimental and theoretical mapping of phonon properties. However, calculations of lattice dynamics at or close to phase transitions in solids are still challenging. On the other hand, corresponding experimental investigations continue to reveal new insights into the driving mechanisms of these phase transitions.
In my talk, I will present our work using phonon spectroscopy in materials featuring electronic phase transitions such as conventional and unconventional superconductivity, nematic order and metal insulator transitions. The results will highlight the strong coupling of phonons to other excitations whereby phonon spectroscopy is able to reveal details on electronic and/or magnetic degrees of freedom.

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Presenter: WEBER, Frank (Karlsruhe Institute of Technology)

Session Classification: Plenary

Track Classification: Plenary

Contribution ID: **172** Type: **Talk (20 min + 5 min discussion)**

Status and Upgrades of the Instruments and the Positron Beam Facility at NEPOMUC

Thursday, December 8, 2022 2:05 PM (25 minutes)

The bright low-energy positron beam provided by the neutron induced positron source in Munich (NEPOMUC) at FRM II is used in a large variety of experiments in materials science, condensed matter and surface physics as well as in fundamental research, e.g., for the creation of a positron-electron pair plasma. Within this contribution, an overview of the current status and developments of the positron beam facility with its instrumentation is given. Plans for the installation of a buffer gas trap for the creation of high-density positron pulses as well ideas for increasing the performance of the remoderated positron bam are elucidated. The upgrades of the positron beam instruments (i) Coincident Doppler-Broadening Spectrometer (CDBS) using a scanning positron micro beam, (ii) instrument for the 2D measurement of the Angular Correlation of Annihilation Radiation (2D-ACAR), and (iii) the surface spectrometer are highlighted. Finally, the planned extension of the positron beam facility and the future operation of positron beam experiments in the experimental hall *East* are presented.

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Presenter: HUGENSCHMIDT, Christoph

Session Classification: Positrons

Track Classification: Positrons