MLZ User Meeting & German Neutron Scattering Conference 2020

Report of Contributions

https://indico.frm2.tum.de/e/um-2020-dn

Contribution ID: **1** Type: **Poster**

The Materials Science group at Heinz Maier-Leibnitz Zentrum (MLZ)

Wednesday, December 9, 2020 2:30 PM (20 minutes)

The Materials Science group consists of more than 50 members recorded in the mailing list and working in a variety of fields related to the applied materials science. Members of this group belong to neutron scattering or positron spectroscopy instruments including the staff acquired through 3rd party funding and the group of fuel cell development. Each month a group meeting is organized to exchange the activities of the group members, especially their scientific work. In the meetings short presentations are given by group members or invited external scientists to introduce the methods and the scientific topics of their studies.
Typical tools applied in the group are diffraction, small-angle scattering, prompt gamma activation analysis, radiography/tomography, inelastic scattering with time of flight method and neutron depth profiling. Besides the development for neutron scattering instrumentation (neutron depth profiling at PGGA instrument, implementation of a testing machine for Stress-Spec and SANS-1 instrument, positron beam experiments, radiography and spectroscopy instruments at ESS) the topics of our scientific studies are: high performance alloys, energy related materials (batteries, hydrogen storage), electronic structure of correlated materials, fundamental properties of plasmas, archeological objects and last but not least the development of a future MEU fuel element for FRM II.

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Presenter: Dr GILLES, Ralph

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **2** Type: **Poster**

Neutron diffraction study of the in-situ tension deformation behaviour of SiCp/Mg-Zn composite

Wednesday, December 9, 2020 3:10 PM (20 minutes)

The work hardening and softening behaviour of SiCp/Mg-5Zn composites influenced by PDZ (particle deformation zone) size were analysed and discussed using neutron diffraction experiment under in-situ tensile deformation at STRESS-SPEC. Peak broadening evolution was interpreted as the modification of dislocation density, which discovered the effect of dislocation on the work hardening behaviour of the composite. For this study, three kinds of PDZ of 5μm, 10 μm, 20 um SiCp/Mg-5Zn composites were fabricated by semi-solid stirring assisted ultrasonic treatment method. The unique tension rig at STRESS-SPEC was used for this at room temperature.
The results show that the work hardening rate of SiCp/Mg-5Zn composites increased with the enlargement of PDZ size, which was attributed to the grain size of SiCp/Mg-5Zn composites increased with the enlargement of PDZ size. Moreover, the stress reduction (ΔPi) values increased continuously during in-situ tensile for SiCp/Mg-5Zn composites due to the stored energy produced during plastic deformation increased, which provided a driving force for the softening effect. The stress reduction (ΔPi) values produced by the softening effect of SiCp/Mg-5Zn composites are affected by the grain size and stored energy produced during in-situ tensile deformation. However, the role of the grain size of SiCp/Mg-5Zn composite on the softening effect is greater than the stored energy.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

In-situ sputter deposition of Al electrodes on active layers of non-fullerene organic solar cells

Wednesday, December 9, 2020 3:30 PM (20 minutes)

Organic solar cells (OSCs) have underwent significant improvements via both, novel organic synthesis and easy fabrication methods. However, the peeling-off of the top electrode fabricated by thermal evaporation (TA) leads to an intrinsic device degradation, which is one of the main reasons for the performance losses of OSCs. TA has the drawback of establishing only a soft contact between the electrode and the functional layer interface. Another disadvantage is the inevitable high temperature during the evaporation process, which can be harmful to organic materials and is energy extensive. To overcome these challenges, the magnetron sputtering technique appears very promising.
For understanding the mechanism of the metal cluster growth, we use in-situ GISAXS to observe the morphology changes during the sputtering process. In detail, the active layer of the organic solar cells is composed of the polymer donor PffDT4T-2OD and the small molecule accepter EH-IDTBR. Both were dissolved in 1,2,4-TMB and CB respectively to obtain different morphologies of the printed films. Then 10 nm MoO3 was deposited on their surface, which acts as the electron blocking layer for the invert solar cell device. A 20 nm Al layer is sputtered ontop as top electrode. Notably, the formation of the Al electrode on MoO3 is slower than on the active layer without deposition of MoO3. In addition, GISAXS, SEM and AFM measurements indicate that the morphology impact on the Al growth significantly.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Phase transition kinetics in a doubly thermo-responsive poly(sulfobetaine)-based block copolymer thin film

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Thermo-responsive polymers show a strong change in volume towards slight changes of their surrounding temperature. While this behavior is well understood for polymers in solution, less is known about the underlying mechanisms in thin film geometry. In our work, we investigate the phase transition kinetics upon increasing temperature in a thermo-responsive block copolymer thin film, that shows both, upper and lower critical solution temperature (UCST and LCST) behavior. Time-of-flight neutron reflectometry (ToF-NR) is used to follow the phase transition kinetics with high time resolution. At temperatures, below the UCST, the polymer film is first swollen in D2O atmosphere to increase the mobility of the polymer chains. Subsequent, temperature is increased to an intermediate regime (between UCST and LCST) and high regime (above LCST). In addition ToF grazing incidence small angle neutron scattering (GISANS) measurements are performed at the beginning and in between the kinetic processes to gain detailed information about the thin film morphology at different temperatures.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Studying the dynamics of PTB7:PCBM blend films with quasielastic neutron scattering

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, a photon is absorbed and an exciton created. After diffusion to a donor-acceptor interface, the exciton is dissipated and charge carriers can be extracted at the electrodes.

A frequently applied and well-studied system is the combination of P3HT ((C10H14S)n) as electron donor and PCBM (C72H14O2) as electron acceptor. Previous studies have shown that internal dynamics and structural layout of the active layer influence its electronic properties and thus its performance in a device.

A more modern, very promising low-band gap electron donor material is PTB7 ((C41H53FO4S4)n). We investigated films of PTB7, PCBM and a mixture of these two, prepared out of chlorobenzene solutions. On these films we performed first quasielastic neutron scattering experiments at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching). Hydrogen dynamics of pure compounds as well as blend films are investigated on a pico- to nanosecond timescale in a temperature range from 150 K to 400 K. Results are compared with the established P3HT:PCBM system.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

In Situ Printing: Insights into the Morphology Formation and Optical Property Evolution of Slot-Die-Coated Active Layers Containing Low Bandgap Polymer Donor and Nonfullerene Small Molecule Acceptor

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Printing of active layers for application in organic solar cells with a meniscus-guided slot-die coating technique is a promising approach to overcome the up-scaling challenge, which is one of the main drawbacks in the field of organic photovoltaics on their way to marketability. Thin films of the conjugated high-efficiency polymer PBDB-T-SF and the non-fullerene small molecule acceptor IT-4F, which can achieve a power conversion efficiency of 13 % are printed with a meniscus-guided slot-die coater. As the solar cell performance is influenced significantly by the morphology of the active layer, it is important to understand the mechanism of structure formation during printing and drying of the active layers to enable a further optimization of the solar cell performance. Meniscus guided slot die coating of PBDB-T-SF:IT-4F is studied in situ with grazing incidence small angle X ray scattering (GISAXS), optical microscopy and UV/Vis spectroscopy to give an insight into the morphology evolution during drying of active layers.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

Identification of Vacancy Defects in Lead Halide Perovskites

Wednesday, December 9, 2020 3:50 PM (20 minutes)

Metal halide perovskites are remarkable optoelectronic materials, within a decade the photovoltaic (PV) power-conversion efficiencies have risen from a few percent to exceed 25%. Yet advance toward the theoretical Shockley-Queisser limit value has slowed and this has been attributed to defect-assisted nonradiative recombination. First-principles calculations provide detailed insight on point defect structure and electronic properties, and on their role in fundamental mechanisms that govern material performance. While experiments have clearly identified the presence of deep defects, there has been no report of an experimental microscopic identification of a point defect. Here we detect and identify the presence of Pb cation monovacancies in the prototypical CH3NH3PbI3 (MAPbI3) using positron lifetime spectroscopy supported by density function theory. Measurements on thin film and single crystal materials all exhibit positron trapping, approaching saturation, to Pb vacancy defects with a density estimated to be greater than ~ 3 x 10^15 cm-3. No trapping to MA cation vacancies was detected. These results demonstrate the capability to experimentally identify and quantify the presence of cation vacancy and vacancy cluster point defects in metal halide perovskite materials.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Angular Distribution of Neutrons Around Thick Beryllium Target of Accelerator-Based 9Be(d, n) Neutron Source

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Experimental work and simulations were carried out to determine the angular distributions of neutrons and yields of the 9Be(d, n) reaction overall angular range (360 deg) on a thick beryllium target as an accelerator-based neutron source at incident-deuteron energy 13.6 MeV. The neutron activation method was used in the experimental part using aluminum and iron foils as detectors to calculate the neutron flux. The Monte Carlo neutral-particles code (MCNP5) was used to demonstrate and simulate the neutron distribution, also to understand and compare it with the experimental results. The neutron energy spectrum was computed using the projection angular-momentum coupled evaporation code PACE4 (LISEþþ) and the spectrum was adopted in MCNP5 code. Two experimental ways were used, one with a beryllium target and another one without the beryllium target, to evaluate the neutron flux emitted only by the beryllium target. Typical computational results were presented and are compared with the previous experimental data to evaluate the computing model as well as the characteristics of emitted neutrons produced by the 9Be(d, n) reaction with a thick Be-target. Moreover, the results can be used to optimize the shielding and collimating system for neutron therapy.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

Hot Neutron Diffraction Experiments under Extreme Conditions on Single Crystals with HEiDi

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Diffraction with neutrons is one of the most versatile tools for detailed structure analysis on various hot topics related to physics, chemistry and mineralogy. The scd HEiDi at the Heinz Maier-Leibnitz Zentrum (MLZ) offers high flux, high resolution and large q range, low absorption and high sensitivity for light elements by using the Hot Source of FRM II.

At very high temperatures studies on Brownmillerite structures as Nd2NiO4+δ and Pr2NiO4+δ concerning their oxygen diffusion pathways reveal anharmonic diplacements of the apical oxygens pointing towards the interstitial vacancy sites which create a quasicontinuous shallow energy diffusion pathway between apical and interstitial oxygen sites [M. Ceretti et al., J. Mater. Chem. A 3, 21140-21148, 2015]. A new DFG project extends these studies including developments on a special mirror furnace to optimize experiments not only at temperatures > 1300K but also in atmospheres with various oxygen contents and different gas pressures are going to reveal more details on this topic.

A recently finished BMBF project shows that studys on tiny samples < 1 mm³ and high pressure (HP) experiments with diamond anvil cells (DAC) can be performed at HEiDi [A. Grzechnik et al.; J. Appl. Cryst. 53 (2020), 1-6]. Also, they can be combined with low temperatures down to 3K. A new BMBF project has been launched in 2019 to improve efficient use of DAC on HEiDi and to build optimized HP cells for other instruments at MLZ (POLI, MIRA, DNS).

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

PUMA: thermal three-axes spectrometer equipped with multi-analyzer and unique polarization option

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In addition to the "normal three axes"mode, PUMA is equipped with the multi-analyzer and -detector setup consisting of 11 arbitrarily configurable analyzer-detector channels suited for kinetic experiments to realize an entire momentum and energy scan in a single shot. Moreover, the same setup can be used also for neutron polarization experiments to determine the spin flip and the non-spin flip components simultaneously at the same state of the sample. Here we show the current status of PUMA with the multi-analyzer setup.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Pretreatment of wood using ionic liquids

Thursday, December 10, 2020 2:45 PM (15 minutes)

In the pretreatment of wood it is essential to apply mild conditions for extracting oligomeric cellulose and possibly lignin that can be used for a variety of environmentally friendly products such as polymers. For this, ionic liquids are ideal due to their mixture of polar and non-polar character, which makes them swelling the wood until it bursts to a rather fluffy material. Using small angle neutron scattering in operando studies, the different states of the pretreatment are identified. After impregnation with the liquid, the cellulose is restructured and forms nano-scale voids. At late stages the cellulose is rather amorphous and quite dilutes. This opens possibilities for enzymatic chain scission in a second step of treatment. The findings are complemented by other techniques, which allows for an optimization of the pretreatment process.

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Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

Structural Properties of Micelles formed by Telechelic Pentablock Quaterpolymers with pH-responsive Midblocks and Thermoresponsive End Blocks in Aqueous Solution

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Stimuli-responsive polymers are of interest for applications in drug delivery or tissue engineering. Telechelic block copolymers, where a pH-responsive midblock is end-capped by thermoresponsive end blocks, have great potential due to their ability to form highly tunable micelles or hydrogels.
In the present work, micelles formed by the telechelic pentablock quaterpolymer P(nBuMA8-*co*-TEGMA8)-*b*-PDMAEMA50-*b*-PEG46-*b*-PDMAEMA50-*b*-P(nBuMA8-*co*-TEGMA8) in dilute aqueous solution are investigated as a function of temperature and pH. The endblocks are statistical copolymers of the thermo-responsive TEGMA (triethylene glycol methyl ether methacrylate) and the hydrophobic nBuMA (*n*-butyl methacrylate). The intermediate PDMAEMA poly(2-(dimethylamino)ethyl methacrylate) block is a weak cationic polyelectrolyte. The hydrophilic poly(ethylene glycol) (PEG) block ensures water-solubility. Using small-angle neutron scattering (SANS) at KWS-1, FRM II, we found that the micelles have a spherical core and a strongly swollen corona. Their aggregation number and size depend sensitively on the pH and temperature. At low temperatures, some polymers form dangling ends, especially at low pH values. With increasing temperature, dangling ends transform into loops at high pH values, while the dangling ends are more abundant at low pH values. In summary, the micelles show complex responsive behavior, including crosstalk between the stimuli.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **13** Type: **Talk**

Design study of a 1-m2 Position Sensitive Neutron Detector (PSND)

Thursday, December 10, 2020 2:45 PM (15 minutes)

Modern Multi-Wire-Proportional-Chambers (MWPC) operating with 10B4C films as solid-state-converter can surpass the performance of ones based on 3He in terms of position resolution and count rate capability at similar detection efficiency [1, 2]. The use of large area coated converters on thin foils forces to develop a mechanical concept to avoid deformations of the neutron sensitive surface due to their own weight and due to acting electrostatic resulting from HV in operation. This concept must allow a parallel stacking of the converter elements in mm distance in order to accumulate conversion efficiency as needed for perpendicular neutron incidence geometry. HZG has introduced [1] and investigated as a contribution to the ESS the idea of stabilizing the converter elements by gas pressure gradient between both sides of the converter to counteract the forces resulting from operation. This concept is applied to the design study of a 1-m2 PSND with a position resolution of 2 mm. The MWPC consists of up to 24x 10B4C coated 0.3 mm thick Aluminum parallel stacked converters with a detection depth < 12 mm each. The deposition method of 10B4C coatings with thicknesses up to 10 µm on pretreated Al substrates was elaborated [2, 3]. The delay-line read-out of the detector coupes for up to 170 kcps per detector plane.
[1] European Patent: EP 17184906.0 (filed at 04.08.2017)
[2] European Patent Application 2 997 174 (14.07.2014)
[3] G. Nowak, et al. J. Appl. Phys. 117, 034901 (2015)

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Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

Contribution ID: **14** Type: **Talk**

Distortion of amphiphile lamellar phases induced by surface roughness

Tuesday, December 8, 2020 1:40 PM (25 minutes)

The structure of concentrated solutions of tetraethyleneglycol dodecyl ether has been compared against a smooth surface and one with a roughness of the order of the lamellar spacing. This has been done in order to investigate the role perturbations have on the overall lamellar order, when these have length scales of the order of the interactions between neighboring lamellae. The results showed that the surfactant forms a well-ordered and aligned structure at a smooth surface, extending to a depth of several micrometers from the interface. Increasing the temperature of the sample and subsequent cooling promotes alignment and increases the number of oriented layers at the surface. The same sample forms a significantly less aligned structure, against a rough surface that does not align to the same extent, even after heating. The perturbation of the structure caused by thermal fluctuations was found to be much less than that imposed by a small surface roughness.

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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **15** Type: **Talk**

Signature of defect-induced symmetry breaking in magnetic neutron scattering

Thursday, December 10, 2020 1:30 PM (15 minutes)

The antisymmetric Dzyaloshinskii-Moriya interaction (DMI) plays a decisive role for the stabilization and control of chirality of skyrmion textures in various magnetic systems exhibiting a noncentrosymmetric crystal structure. A less studied aspect of the DMI is that this interaction is believed to be operative in the vicinity of lattice imperfections in crystalline magnetic materials, due to the local structural inversion symmetry breaking. If this scenario leads to an effect of sizable magnitude, it implies that the DMI introduces chirality into a very large class of magnetic materials—defect-rich systems such as polycrystalline magnets. Here, we show experimentally that the microstructural-defect-induced DMI gives rise to a polarization-dependent asymmetric term in the small-angle neutron scattering (SANS) cross section of polycrystalline ferromagnets. The results are supported by theoretical predictions using the continuum theory of micromagnetics. This effect, conjectured already by Arrott in 1963, is demonstrated for nanocrystalline terbium and holmium (with a large grain-boundary density), and for mechanically-deformed microcrystalline cobalt (with a large dislocation density). Analysis of the scattering asymmetry allows one to determine the defect-induced DMI constant, $D = 0.45 \pm 0.07\,\mathrm{mJ/m^2}$ for Tb at $100\,\mathrm{K}$. Our study proves the generic relevance of the DMI for the magnetic microstructure of defect-rich ferromagnets.

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Presenter: Prof. MICHELS, Andreas (University of Luxembourg)

Session Classification: DN2020: Magnetism

Track Classification: DN: Magnetism

Contribution ID: **16** Type: **Poster**

Complementarity of PNR and XMCD for monolayer-magnetism in hetero-epitaxial Fe on Cu(001)

Wednesday, December 9, 2020 5:40 PM (20 minutes)

We have combined two complementary techniques, element sensitive ex situ X-ray magnetic circular dichroism (XMCD) and in situ polarized neutron reflectivity (i-PNR), to determine the values of evolving magnetic moments obtained from a low symmetry system of hetero-epitaxial Fe monolayers (MLs), as a function of thickness. The samples were grown by magnetron sputtering on face-centered-cubic (fcc) Cu(001)/Si(001). Within experimental errors, we found a corroboration of the modulated moments from the XMCD and of the magnetic anisotropies from magnetization measurements with those obtained earlier from layer-by-layer i-PNR measurements. Furthermore, analyzing the depth sensitive i-PNR profile of a bulk-like film, we developed a model characterized by monotonic magnetism involving collinear spins. The results have been compared with those existing, following the theoretical parameterized tight-binding model with satisfactory agreement. This study distinguishes the variation of monolayer-magnetism owing to the growth morphology from the layer-by-layer investigation vis-à-vis depth-profiling of bulk-like film. At the same time, it also promises the general possibility of depth-profiling using i-PNR in other complex multilayered systems on high flux neutron sources.

Journal of Magnetism and Magnetic Materials 505 (2020) 166701 https://doi.org/10.1016/j.jmmm.2020.166701

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

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

Surface distortion of Fe dot-decorated TiO2 nanotubular templates using time-of-flight grazing incidence small angle scattering

Wednesday, December 9, 2020 4:10 PM (20 minutes)

Physical properties of nanoclusters, nanostructures and self-assembled nanodots, which in turn are concomitantly dependent upon the morphological properties, can be modulated for functional purposes. Here, in this article, magnetic nanodots of Fe on semiconductor TiO2 nanotubes (TNTs) are investigated with time-of-flight grazing incidence small-angle neutron scattering (TOF-GISANS) as a function of wavelength, chosen from a set of three TNT templates with different correlation lengths. The results are found corroborating with the localized scanning electron microscopy (SEM) images. As we probe the inside and the near-surface region of the Fe-dotted TNTs with respect to their homogeneity, surface distortion and long-range order using TOF-GISANS, gradual aberrations at the top of the near-surface region are identified. Magnetization measurements as a function of temperature and field do not show a typical ferromagnetic behavior but rather a supermagnetic one that is expected from a nonhomogeneous distribution of Fe–dots in the intertubular crevasses.
Scientific Reports | (2020) 10:4038 | https://doi.org/10.1038/s41598-020-60899-2

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Presenter: PAUL, Amitesh

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **18** Type: **Poster**

KWS-1 SANS instrument with polarization analysis

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The KWS-1 small-angle neutron scattering instrument is operated by JCNS at MLZ [1]. The instrument covers a q-range from 0.0007 to 0.5 $Å^{-1}$ with a selectable wavelength span from 4.7 to 20 Å. The maximum neutron flux on the sample is 1×10^{8} cm^{-2} s^{-1}, making it one of the most intense SANS instruments in the world.

The instrument is equipped with transmission supermirror polarizer, adiabatic radio-frequency spin flipper and a recently obtained dedicated magnet and polarization analyzer. The three-channel V-cavity polarizer with Fe/Si coated supermirrors (m=3.6) has an average polarization >93% and is positioned in a custom designed changer of revolver type. The flipper provides a high flipping efficiency of more than 99.9% for all neutron wavelengths. A custom designed hexapod allows heavy loads and precise sample positioning in beam (also for grazing incidence SANS under an applied magnetic field). For the experiments with the polarization analysis a 3He analyzer is utilized. The new sample magnet allows close positioning of the ^{3}He cell to the magnet. The magnet has two orthogonal horizontal accesses. For the maximum field of 3 T (parallel to the beam) the decay time, T1, of the ^{3}He cell approximately 50 cm away from the center of the magnet constituted 90 hours. The maximum analyzed q is 0.06 $Å^{-1}$.

All instrument components are running under a flexible instrument control system (NICOS).

[1] A.Feoktystov, H.Frielinghaus, Z.Di, et al., J. Appl. Cryst., 48, 61 (2015)

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Structural characterization and rheology of bio-compatible wormlike micelles

Thursday, December 10, 2020 2:15 PM (15 minutes)

Wormlike micelles exhibit a unique viscoelastic behavior, which has been investigated intensely in the past decades, experimentally as well as by theoretical calculations [1,2]. Within our studies we explore the self-assembled structure and the flow behavior of wormlike micelles formed by mixing a short-chained C_8 cationic surfactant and the sodium salts of omega-9 fatty acids [3]. Within the class of the latter one, the alkyl chain length is varied from C_{18} to C_{22}, yielding an increase of the micellar cross section. The structure of the micelles is characterized by neutron scattering experiments. Beside the thickness of the micelles the persistence length is an important key quantity which strongly influences the flowing properties and is depending on the mixing ratio of both surfactants. Further, it is observed that the dynamical response, i.e., the time scales such as the relaxation or breakage time, of the micelles is influenced by the molecular architecture. Combining the results of rheological measurements with the neutron scattering experiments allows us to get a detailed insight into the micellar structure and dynamics.

[1] C. Dreiss, Soft Matter **3**, 956, (2007)
[2] P. D. Olmsted, Rheo. Acta **47**, 283, (2008)
[3] Raghavan *et al.*, Langmuir **18**, 3797 (2002)

Primary author: VON LOSPICHL, Benjamin (Technische Universität Berlin)

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Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

Contribution ID: **20** Type: **Talk**

High resolution neutron spectroscopy with the J-NSE ”PHOENIX”

Thursday, December 10, 2020 1:45 PM (15 minutes)

Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. In terms of Fourier-time (τ) high resolution means the extension of τ into to the regime of μs (corresponding to an energy resolution of ~neV). The J-NSE “PHOENIX” with its unique fringe-field compensated, superconducting magnets provides the state of the art in NSE instrument design. One of the most innovative characteristics of the coils is their optimized geometry that maximizes the intrinsic field-integral homogeneity along the flight-path of the neutrons and that enhances the resolution of a factor 2.5 compared to the previous normal conducting setup. The increased resolution may be exploited to reach larger Fourier-times and/or to benefit from significant intensity gains if shorter neutron wavelengths are used at a given Fourier-time. Thus the J-NSE “PHOENIX” meets the needs to look into the microscopic dynamics of soft- or –biological matter with enhanced and new quality. Here we present the results on the performance of the spectrometer in its current configuration and some selected examples from the realm of soft matter dynamics that exploit the unique properties of the new J-NSE.

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Presenter: HOLDERER, Olaf

Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

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

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

Wednesday, December 9, 2020 4:50 PM (20 minutes)

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

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **22** Type: **Poster**

Germanium-based nanostructure synthesis guided by amphiphilic diblock copolymer templating

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Latest research in the field of hybrid photovoltaics focuses on the benefits of inorganic and organic materials. Flexibility, low cost and large-scale production are the most valuable properties of organic components whereas the inorganic components add chemical and physical stability. So far thin films based on titanium dioxide are well investigated, whereas less is known about germanium-based compounds. In this work, we analyze thin films with optical, electrical and morphological measurement techniques to understand and control the corresponding properties. An amphiphilic diblock copolymer templating with polystyrene-b-polyethylene oxide (PS-b-PEO) and a metal-semiconductor precursor are used to prepare thin films via sol-gel synthesis. The copolymer templating results in nanoporous foam-like germanium-based thin films. In the present study, thin films with different polymers with varied molar weights of polystyrene and polyethylene oxide are prepared and analyzed. As the major technique for real-space imaging in this research field, SEM can only provide information about the surface. Therefore grazing incidence small angle X-ray scattering (GISAXS) experiments are carried out and have to be validated with grazing incidence small angle neutron scattering (GISANS) to understand the formation of the inner structure morphology.

Primary authors: WEINDL, Christian L. (TUM Physik); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Prof. FÄSSLER, Thomas F.; FAJMAN, Christian

Presenter: WEINDL, Christian L. (TUM Physik)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

Dehydration of thermoresponsive molecular brushes with block or random copolymer side chains

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Molecular brushes with thermoresponsive copolymer side chains have attracted attention for drug delivery purposes because of their elongated shape and their versatility. In the present work, two molecular brushes having copolymer side chains composed of poly(propylene oxide) (P) and poly(ethylene oxide) (E) are studied in aqueous solution. The side chains are either a diblock (PbE) or a random copolymer (PrE). Their structures, dehydration and aggregation behavior around the cloud point, Tcp, are investigated using small-angle neutron scattering (SANS) at KWS-1, MLZ [1].

At 25 ℃, the brushes are elongated and feature a core-shell structure with a polymer-rich core and a water-rich shell. Upon heating to Tcp, PbE dehydrates only weakly, and the shell shrinks slightly. Above Tcp, large aggregates from strongly interpenetrating brushes are formed, which is due to the high mobility of the still rather hydrated side chains. In contrast, PrE undergoes a rod-to-disk shape transformation along with a severe decrease of the water content, already before aggregation sets in at Tcp. Above, the PrE brushes form small aggregates from loosely connected brushes, which is a result of the low side chain mobility. Thus, the choice of the side chain architecture not only allows control of the inner structure and shape, but also of the transition behavior.

[1] J.-J. Kang, C. M. Papadakis et al., *Macromolecules* **53**, 4068 (2020)

Primary author: KANG, Jia-Jhen (Physik-Department, Technische Universität München)

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

CSPEC- a cold time of flight spectrometer for the ESS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The European Spallation Source (ESS) is expected to be the world's most powerful neutron source. Among the endorsed instruments foreseen for day one instrumentation at ESS, is the cold time-of-flight spectrometer CSPEC, collaboration between the Technische Universität München, and the Laboratoire Léon Brillouin. CSPEC will probe the structures, dynamics, and functionality of large hierarchical systems as they change or operate. Hierarchical systems include liquids, colloids, polymers, foams, gels, and granular and biological materials as well as the ever-complex low-energy dynamics of energy and magnetic materials. The unique pulse structure of the ESS with its long pulse duration (2.86 ms) and a repetition rate of 14 Hz requires new concepts for the instrumentation to make optimum use of the available source time frame. The energy resolution can be tuned in the range of ΔE/E = 6 - 1%, and CSPEC will utilize cold neutrons in the range from λ = 2 - 20 Å with the focus on the cold part of the spectrum. The large detector area, with a radius of 3.5 m, 5 −140 degrees and 3.5 m in height, typical on a chopper spectrometer will be designed with optimal energy and Q resolution in mind while maintaining the highest signal to noise ratio. CSPEC is now in the detailed design phase, and we will present the current status and the expected performance.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **25** Type: **Talk**

Dynamics of porous and amorphous magnesium borohydride to understand solid state Mg-ion-conductors

Thursday, December 10, 2020 3:45 PM (15 minutes)

Rechargeable solid-state magnesium batteries are considered for high energy density storage and usage in mobile applications as well as to store energy from intermittent energy sources. Recently, magnesium borohydride, $Mg(BH_4)_2$, was found to be an effective precursor for solid-state Mg-ion conductors. The mechanochemical synthesis tends to form amorphous $Mg(BH_4)_2$ and it has been postulated that amorphous $Mg(BH_4)_2$ is increasing the conductivity in the Mg-ion conductors. Quasi-elastic neutron scattering (QENS) studies were employed to investigate the dynamics of porous and amorphous $Mg(BH_4)_2$. In general, QENS is needed to understand the local structure and dynamics in the precursor at different temperatures as well as at different energy- and momentum transfers. The results show that the low energy excitation spectrum in $Mg(BH_4)_2$ is strongly dependent on the local structure as can be seen by the comparison of as-received γ-$Mg(BH_4)_2$ and ball milled, amorphous compound. While as-received γ-$Mg(BH_4)_2$ shows almost no quasi-elastic scattering at 310 K, the ball milled version displays a significantly different low energy excitation spectrum and a higher rotational mobility of the [BH4] units. A high rotational mobility is proposed to be a fundamental necessity for high Mg-ion conductivity. This is supported by an almost two orders of magnitude higher conductivity in the ball milled sample compared to the as-received γ-$Mg(BH_4)_2$ at 353 K.

Primary authors: LOHSTROH, Wiebke (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München); HEERE, Michael (Institute for Applied Materials—Energy Storage Systems (IAM-ESS), Karlsruhe Institute of Technology (KIT))

Presenter: LOHSTROH, Wiebke (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

Session Classification: DN2020: Materials

Track Classification: DN: Materials

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

Phase Transformation in AlTiNbVW High Entropy alloy

Wednesday, December 9, 2020 5:10 PM (20 minutes)

High entropy alloys (HEAs), which comprise more than five principal elements, are presently of great interest in materials science and engineering. A predication by CALPHAD has been performed in a new AlTiNbVW HEA, which shows that this alloy consists of two similar bcc phases in the as-cast condition. Current work is to study the phase composition in this multicomponent alloy system at equiatomic condition using neutron/synchrotron diffraction under heat treatment. The chemical composition and microstructure of these two bcc phases has been determined using Energy Dispersive X-Ray Analysis (EDX) and Backscattered-Electron (BSE) Imaging. A diffusion controlled phase transformation between these two bcc phases has been found to take place between 1000℃ and 1700℃. The phase transformations kinetic of this bcc1 to bcc2 transformation has been studied systematically using in-situ neutron/synchrotron diffraction with combination of a dilatometer.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

The relevance of protein dynamics for protein folding: The case of apomyoglobin

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Dynamics of different folding intermediates and denatured states might have implications in understanding protein folding. Apomyoglobin (apoMb) has been investigated using neutron spin-echo spectroscopy (NSE) and SANS [1] and quasielastic neutron scattering (QENS) [2,3] in different states: native-like, partially folded and completely unfolded. Mean square displacements obtained by QENS showed a correlation with the secondary structure content of apoMb [2,3]. However, recent NSE & SANS data offered a detailed picture on the physical nature of slow collective dynamics and different dynamics behavior was observed [1]. While the internal dynamics of the native-like state can be understood using normal mode analysis based on high resolution structural information of myoglobin, for the unfolded and even for the molten globule states, models from polymer science are employed. The Zimm model accurately describes the slowly-relaxing, expanded GdmCl-denaturated state. Dynamics of the acid unfolded and molten globule state are similar in the framework of the Zimm model with internal friction. Transient formation of secondary structure elements in the acid unfolded and presence of α-helices in the molten globule state lead to internal friction to a similar extent, which demonstrates the importance of secondary structure elements as source of internal friction in partially folded proteins.

1. Balacescu et al. Scie Rep, 2020
2. Stadler et al. JPCB, 2015
3. Stadler et al. PCCP, 2016

Primary authors: BALACESCU, Livia (RWTH Aachen); SCHRADER, Tobias; RADULESCU, Aurel (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ); ZOLNIERCZUK, Piotr; HOLDERER, Olaf; PASINI, Stefano (Forschungszentrum Juelich GmbH); FITTER, Joerg; STADLER, Andreas (FZ Jülich)

Presenter: STADLER, Andreas (FZ Jülich)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Localized strain induced abnormal growth of cube oriented grain in a graphene nanosheets (GNS) reinforced copper matrix composite

Wednesday, December 9, 2020 4:30 PM (20 minutes)

Graphene nanosheets (GNS) reinforced copper (Cu) matrix composites were fabricated through electrophoretic deposition (EPD) and vacuum hot-pressing sintering process. The bulk texture of the as-sintered pure Cu and the GNS/Cu shows that a strong cube component formed in the GNS/Cu, while the pure Cu sintered with the same method exhibits coarse grains with random orientations. Thereafter, the evolution of microstructure and texture during sintering were characterized by SEM-EBSD and neutron diffraction ex-situ, and the macro and local strain of Cu during the sintering process was investigated in-situ using a dilatometer at high energy synchrotron radiation source at HEMS, DESY. The primary results indicate that the micro strain in the GNS/Cu which contributed by the thermal expansion mismatch between GNS and Cu during sintering can enhance the growth of the cube oriented grains, which finally lead to a strong cube texture inside the GNS/Cu composite.

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Presenter: SHI, Hailong

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **29** Type: **Talk**

Learning from structure solution: An enhanced solid-state Mg electrolyte

Tuesday, December 8, 2020 3:25 PM (25 minutes)

All-solid-state batteries based on magnesium are considered for the use in mobile applications as well as to store energy from "renewable"intermittent energy sources. Recently, a solid state magnesium ion conductor, Mg(en)1(BH4)2 (en stands for ethylenediamine), obtained from Mg(BH4)2 : [Mg(en)3(BH4)2] 2:1 mixture, was reported to have an exceptionally high magnesium ion conductivity of up to 6·10−5 S·cm−1 at 70 ℃. Here we show that this synthesis actually yields a mixture of Mg(en)1.2(BH4)2 and amorphous Mg(BH4)2. The latter was often neglected in previous investigations, though it was shown recently that its dynamics have a positive influence on the conductivity. The structure of Mg(en)1.2(BH4)2 has been solved from single crystal X-ray diffraction in space group P-1 and confirmed by neutron powder diffraction on isotopically substituted Mg(en)1.2(11BD4)2. Its structure shows three Mg atoms with coordination numbers 4, 5 and 6, the BH4 groups behaving as terminal and bridging ligands, and en chelating and bridging Mg atoms. This complexity makes the structure solution virtually impossible from powder diffraction data. Thermal decomposition of Mg(en)1.2(BH4)2 goes through an intermediate formation of the previously unknown Mg(en)2(BH4)2, its structure was solved from synchrotron X-ray powder diffraction, complemented by DFT optimization.

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Presenter: HEERE, Michael

Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

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

New primary optics for the ʻEnergy research with Neutronsʼ option at MLZ.

Thursday, December 10, 2020 2:00 PM (15 minutes)

The Energy research with Neutrons (ErwiN) instrument is meant to be used for the investigation of energy storage materials, also integrated in complete components and under real operating conditions. Thus, it is possible to scan a large parameter space (e.g. temperature, state of charge, charge rate, fatigue degree) for the investigation of modern functional materials in kinetic and time-resolved experiments. Diffraction data will be obtained from the entire sample volume or in a spatially resolved mode from individual parts of the sample.
The future development of the ErwiN instrument is presented here: Firstly, the plans of replacing the primary beam optics will be revealed to bring this diffractometer to the same level as the high flux and high resolution instrument D20 at the ILL. The upgraded ErwiN is designed for different scenarios: for very fast measurements at medium resolution, for medium fast measurements at higher resolution and also for very high resolutions still at reasonable velocity. The commissioning and integration of ErwiN will enhance the attractiveness for a wider community in energy research as well as materials science while novel methods for the neutron science community will be developed.

Primary authors: HEERE, Michael; SENYSHYN, Anatoliy; EHRENBERG, Helmut (KIT); KNAPP, Michael (KIT, IAM-ESS)

Presenter: HEERE, Michael

Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

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

Commissioning of the ʻEnergy research with Neutronsʼ option at MLZ.

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The Energy research with Neutrons (ErwiN) instrument is meant to be used for the investigation of energy storage materials, also integrated in complete components and under real operating conditions. Thus, it is possible to scan a large parameter space (e.g. temperature, state of charge, charge rate, fatigue degree) for the investigation of modern functional materials in kinetic and time-resolved experiments. Diffraction data will be obtained from the entire sample volume or in a spatially resolved mode from individual parts of the sample.
The commissioning of the ErwiN instrument is presented here. The commissioning and integration of ErwiN will enhance the attractiveness for a wider community in energy research as well as materials science while novel methods for the neutron science community will be developed.

Primary authors: HEERE, Michael; SENYSHYN, Anatoliy

Presenter: HEERE, Michael

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Quantum Phenomena

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

The Myelin Basic Protein and its Phase Behaviour

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The Myelin Basic Protein (MBP) is an essential part of the myelin sheath in almost all vertebrates and, thus, contributes significantly to flawless signal conduction. Here, one of its key properties is the ability to perform a Liquid-Liquid Phase Separation (LLPS), the coexistence of highly concentrated protein phases within a diluted solution.
Microscopy experiments indicated that a LLPS would occur upon the addition of Polyethylene glycol (PEG). By using contrast matched PEG in 100% D2O, USANS experiments at KWS-3 in MLZ confirmed that the optically observed droplets originated from MBP condensates. The droplet size was determined to be in the low µm range, which is in good accordance with DLS measurements. Kinetic studies on the droplet growth have pointed out that an equilibrium size was reached after only a few minutes. Furthermore, the investigations have shown that both coalescence and Ostwald ripening contribute to droplet expansion.
Neutron scattering experiments at KWS-2 revealed unfolding of the proteins as well as increasing size of single MBP molecules upon the addition of PEG. As a complementary technique, CD spectroscopy was used which supported the previous finding.
It is concluded that variations of protein structure and the occurrence of a LLPS are related phenomena which affect each other. Hence, future examinations will cover this effect in detail, as well as droplet growth kinetics of the earliest stages of a LLPS with improved temporal resolution.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

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

Calibration of p-XRF on ancient pottery using NAA results

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The chemical fingerprint of a representative corpus of sherds from Central Europe, North Africa, Western and Central Asia was identified by using neutron activation analysis (NAA) at the FRM II. A first batch of 30 homogenized pottery samples from archaeological field projects of LMU researchers were analysed using standard procedures following both short and long-time irradiation and measured on gamma-detectors after different decay times. 40 elements incl. many trace elements could be determined. The NAA results were then compared with the results of portable XRF instruments which are routinely used on archaeological excavations in Germany and abroad. Properly calibrated with securely identified reference material such portable equipment allows for the serial screening of ancient pottery, which in turn informs us on raw material acquisition, production cycles and, ultimately, the role of imports and the supply networks of a given society. The set of analyses carried out therefore constitutes an important step in the improvement of a research methodology. The FRM II samples will constitute the basis of a specialized calibration for ancient pottery analysis that shall subsequently be established as reference standard for other laboratories and researchers working with p-XRF.

Primary authors: SCHAUER, Michaela (LMU München); LI, Xiaosong (TUM/FRM II); Dr KANIUTH, Kai (Vorderasiatische Archäologie LMU)

Presenter: SCHAUER, Michaela (LMU München)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Oscillatory dynamics in simple systems at elevated temperatures – beyond a perturbational treatment of anharmonicity

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The importance of anharmonicity for describing fundamental materials properties, starting from finite heat conductivity due to phonon-phonon scattering, can hardly be overemphasized. For crystalline matter, the principal microscopic gauge is constituted by the broadening in energy of the phonon dispersions, corresponding to q-dependent phonon lifetimes, which is also the main unknown for microscopic computations of heat conductivity.

Here the case of elemental Al at temperatures up to the melting point will be considered. I will present experimental data obtained by inelastic neutron scattering with consideration to the necessary steps in data analysis for being able to extract the inherent linewidths. Further, I will present calculations of q-dependent line broadenings on the basis of density-functional theory, both in the standard approach of perturbation theory as well as via ab initio molecular dynamics, and I will discuss why perturbation theory fails at elevated temperatures.

A. Glensk et al., *Phys. Rev. Lett.* **123**, 235501 (2019)

Primary author: LEITNER, Michael

Presenter: LEITNER, Michael

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Materials

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

Temperature-dependent Phase Behavior of the Thermoresponsive Polymer Poly(N-isopropylmethacrylamide) in Aqueous Solution

Wednesday, December 9, 2020 5:35 PM (25 minutes)

Compared to the widely-investigated poly(N-isopropylacrylamide) (PNIPAM), poly(N-isopropylmethacrylamide) (PNIPMAM) has a higher phase transition temperature (43 ℃ instead of 32 ℃). PNIPMAM has a similar chemical structure as PNIPAM, but the additional methyl groups on its backbone may lead to steric hindrance and weaker intramolecular interactions. To understand how these effects affect the thermal and structural behavior of PNIPMAM aqueous solutions, we investigate the phase behavior of PNIPMAM in D2O using turbidimetry, differential scanning calorimetry, Raman spectroscopy, small-angle and very small-angle neutron scattering (at KWS-1 and KWS-3 at MLZ). The PNIPMAM solutions undergo first macroscopic phase transition, but the PNIPMAM chains only dehydrate 2~3 ℃ above TCP. The methyl groups in PNIPMAM give rise to a more compact local chain conformation than in PNIPAM. Moreover, physical crosslinks and loosely packed large-scale inhomogeneities and physical crosslinks appear already in the one-phase state. We assign these differences to enhanced attractive intermolecular interactions resulting from the hydrophobic methyl groups. In the two-phase state, PNIPMAM mesoglobules are larger and more hydrated than PNIPAM mesoglobules. This is attributed to the steric hindrance caused by the methyl groups, which weaken the intrapolymer interactions. Thus, the methyl groups in PNIPMAM chains play a crucial role in the thermal and structural behavior around the phase transition.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **38** Type: **Poster**

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

REFSANS is the horizontal ToF reflectometer at the MLZ in Garching. It is designed to carry out specular and off-specular reflectivity, as well as GISANS studies of solid/liquid, solid/air and liquid/air interfaces. Through ToF analysis, REFSANS gives simultaneous access to a range of Q values (with Qmax/Qmin up to ≈ 7), useful to study air-liquid interfaces and kinetic phenomena.
A chopper-system composed by six disks allows a tunable wavelength resolution, from 0.2 % up to 10%. The neutron optics of REFSANS 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.
Given the ToF nature of REFSANS, the investigation of kinetic processes is based on the possibility to embrace a Q-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 after the experiment. Beside the typical sample environment, a three-electrode electrochemical compact cell was recently realized for investigation of phenomena at the electrode surface. Currently, the design of a humidity cell is in progress, to allow investigations of processes in a controlled atmosphere.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

KWS-2 the high Intensity / wide Q-range SANS diffractometer

Wednesday, December 9, 2020 5:40 PM (20 minutes)

KWS-2 is a classical SANS diffractometer using a combination of pinholes with different neutron-wavelengths and detector distances as well as a focusing mode with MGF2 lenses to reach a large q-range between 0.0002 and 0.5 1/Å. A wide-angle detection option is currently planned to allow for measurements up to 2 1/Å, by combining SANS and WANS methods.
The instrument is designed for high intensity studies with a broad q-range, covering mesoscopic structures and their changes due to kinetic processes in the fields of soft condensed matter, chemistry, and biology.
The high neutron flux and the possibility to measure samples with large diameter (up to 5 cm), employing lenses, allow for high intensity and time-resolved studies.
In special cases, the resolution can be improved by using a double-disc chopper with adjustable openings reaching a wavelength spread between 2 and 20 %. In this way, the instrument can be flexibly adjusted to the needs of different experiments. Furthermore, the effects of chromatic aberration of the lenses and gravitation effects can be minimized. By using a secondary single-disc compact chopper, the use of the TOF mode achieves a good separation of the elastically, quasi-elastically and inelastically scattered neutrons from the sample. When only the quasi-elastic scattered neutrons are considered for the data analysis, a lower background level is obtained at high q, which makes the measurement of weak coherent signals more reliable.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **40** Type: **Talk**

Nanoscale Structural Rearrangements in Ultrathin Nanocellulose Films induced by Water

Tuesday, December 8, 2020 2:05 PM (25 minutes)

Cellulose nanofibrils (CNF) as a sustainable biomaterial are excellent building blocks for mechanically exceptional materials and functional coatings. Yet, the water uptake and response to humidity still poses a challenge. We first demonstrate a facile route to prepare large-scale cellulose-based nanostructured thin films with a low surface roughness down to 2.5 nm on (20 × 100) mm^2 substrates. We employ in situ grazing incidence small-angle neutron scattering to study the morphological features within the ultra-smooth CNF thin films under as-prepared conditions as well as their rearrangement under humidification. Increasing CNF surface charge is highly beneficial for the layering mechanism as it directly influences the self-assembly process, which results in a low roughness of the densely packed CNF network. We observe distinct domains of smaller cellulose bundles and larger bundles or agglomerates within the thin film. During in situ humidification and drying of the CNF film, the domains reversibly change from cylindrical to spherical appearance. With decreasing values of surface roughness corresponding to increasing surface charge densities of CNF films, the surface free energy is observed to be tunable. This knowledge can be used to promote the use of polar solvents in applications such as organic solar cells and to further enhance physical properties and materials lifetime.

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Presenter: ROTH, Stephan (DESY / KTH)

Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

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

Influence of benzocaine, propranolol and cholesterol on phospholipid bilayers

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Cell membranes play a fundamental role in protecting the cell from its surroundings, in addition to hosting many proteins with fundamental biological tasks. Drugs are able to perturb the structure of cell membranes, which can ultimately give rise to undesirable effects. Thus, a study of drug/lipid interactions is a necessary and important step in fully clarifying the role and action mechanism of active ingredients, and shedding light on possible complications caused by drug overdosage. Here we present the results obtained in our research focused on the understanding of the influence of benzocaine and propranolol active principles on the structure of L-□-phosphatidylcholine-based membranes. The investigation has been performed by means of neutron reflectivity, grazing incidence small angle neutron scattering, and small/ultra-small angle neutron scattering.
Investigations allowed discovering a stiffening of the membranes and the formation of stalks, caused by the presence of benzocaine: the addition of cholesterol increases the amount of stalks formed, if it is present up to a certain percentage (around 10% in mol). On the other hand, disordered bilayers (lamellar powders) and highly curved structures were found in the presence of propranolol. The results obtained may be rationalized in terms of the molecular structures of drugs and may serve as a starting point for explaining the toxic behavior in long-term and overdosage scenarios.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

The strengths of small-angle neutron scattering for magnetic nanoparticle characterization

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In this talk, we will present our recent advances in applying magnetic small-angle neutron scattering (SANS) for the in-depth characterization of magnetic nanoparticles.
In the first part, we will discuss the benefits of a Bayesian analysis as the new standard for fitting magnetic SANS data of nanoparticle samples [1]. Such a standardized protocol for the refinement of magnetic SANS data is especially useful with biomedical applications of magnetic nanoparticles in mind, as regulatory work regarding prior particle characterization is required to guarantee a safe and effective administration of the particles into the human body.
In the second part, we will demonstrate the unique ability of magnetic SANS to detect very small deviations of the magnetization configuration from the homogeneously magnetized state within nanoparticle (NP) systems [2,3]. The SANS technique has been already used in several other studies to investigate the intra- and interparticle magnetization profile in various NP systems. However, in contrast to the previous works, our analysis is focused on model-independent approaches. Moreover, we employ large-scale micromagnetic continuum simulations to support our findings and to disclose the delicate interplay between the particle size and the magnetization profile within NPs.

[1] Bersweiler *et al.*, Nanotechnology, in press (2020)
[2] Bersweiler *et al.* PRB **100**, 144434 (2019)
[3] Vivas *et al.* arXiv:2003.08694 (2020)

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Presenter: BERSWEILER, Mathias (University of Luxembourg)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

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

TOFTOF –cold neutron time-of-flight spectrometer

Wednesday, December 9, 2020 5:40 PM (20 minutes)

TOFTOF is a direct geometry disc-chopper timeof-flight spectrometer located in the Neutron Guide Hall West. It is suitable for both inelastic and quasielastic neutron scattering and the scientific questions addressed range from the dynamics in disordered materials in hard and soft condensed matter systems (such as polymer melts, glasses, molecular liquids, or liquid metal alloys), properties of new hydrogen storage materials to low-energy magnetic excitations in multiferroic compounds, and molecular magnets.
A cascade of seven fast rotating disc choppers which are housed in four chopper vessels is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging supermirror 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 (up to 22 000 rpm) 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.

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Presenter: WOLF, Marcell (TUM)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **44** Type: **Talk**

Adaptive microgels: to squeeze or not to squeeze?

Thursday, December 10, 2020 3:30 PM (15 minutes)

Microgels are macromolecular networks swollen by the solvent they are dissolved in. They are unique systems that are distinctly different from common colloids, such as, e.g., rigid nanoparticles, flexible macromolecules, micelles or vesicles. When swollen, they are soft and have a fuzzy surface with dangling chains and the presence of cross-links provides structural integrity. They find applications e.g., in biocatalysis and as sensors.
At high packing density, microgels can deswell, interpenetrate and deform, thus they can behave like particles or / and macromolecules. Due their properties, microgels can be used to tune the particle-to-polymer transition.
We will discuss properties of microgels of different architectures both in aqueous solution and at interfaces. In particular we will address ultra-low cross-linked microgels, hollow and anisotropic microgels which are sensitive to stimuli as, e.g. temperature and pH.
The structure of microgels is investigated by means of scattering methods, especially exploiting the technique of contrast variation in small angle neutron scattering. The results will be compared to data obtained from super resolved fluorescence microscopy, scanning force microscopy and computer simulations.

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Brugnoni, M.; et al Polym. Chem. 2019, 10, 2397.

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Presenter: RICHTERING, Walter (RWTH Aachen)

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

A study of Linear and Nonlinear Aging in Lithium-Ion Cells by Neutron Diffraction

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Commercial 18650-type C/LiNi0.33Mn0.33Co0.33O2 lithium-ion cells were exposed to different charging, discharging and resting conditiones to understand their influence on the aging behaviour. When cycled with a standard 1C charging and discharging rate and different resting times, the cells show a nonlinear capacity fade after a few hundred equivalent full cycles. By increasing the discharging current or decreasing the charging current, the lifetime improves and results in a linear capacity fade. The neutron diffraction experiment reveals a loss of lithium inventory as the dominant aging mechanism for both linearly and nonlinearly-aged cells. No structural degradation of electrode materials, or their deactivation was seen. With ongoing aging, we observe an increasing capacity loss in the edge area of the electrodes. Whereas the growth of the solid electrolyte interphase defines the early stage, linear aging, marginal lithium deposition is supposed to cause the later stage, nonlinear aging.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **46** Type: **Talk**

Dynamics during an arrested phase transition in a protein system

Thursday, December 10, 2020 2:30 PM (15 minutes)

Phase separation in biological systems is a path for the formation of cellular organelles[1]. To understand the dynamic properties of these compounds we studied a protein solution model system during the phase separation with neutron spin-echo and back scattering spectroscopy as well as with small angle scattering. The phase separation for the investigated sample occurs for temperatures below T_p= 21°C and is due to the short-range depletion interaction induced by a polymer (polyethylene glycol). The evolution of the phase separation after a quench to temperatures below T_p was monitored though the scattered intensity measured with small angle scattering[2]. For quenches to temperature to 6°C and below the phase separation arrests. This phenomenon was previously linked to the dynamical arrest at molecular length scale due to gelation[3]. The collective diffusion agrees with anomalous diffusion and relaxation times which are two orders of magnitude smaller in the arrested state. Using back scattering we can monitor the polymers and proteins self-diffusion, showing Brownian motion on the diffusive short-time scale even in the arrested state, and a significant transition of the protein diffusion when crossing the phase separation temperature.
[1] Berry, J., Brangwynne, P. C. & Haataja, M. , Reports on Progress in Physics 81, 046601 (2018).
[2] Da Vela, S. et al., Soft Matter 13, 8756-8765 (2017).
[3] Zaccarelli, E., J. Phys.: Cond. Matter 19, 323101 (2007).

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Presenter: GIRELLI, Anita

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

Contribution ID: **47** Type: **Talk**

Conducting polymer infiltration in porous cellulose thin films

Thursday, December 10, 2020 4:15 PM (15 minutes)

Cellulose nanofibrils (CNF) have proven their strengths in conductive and transparent films. A promising route for fabricating porous CNF films on large scale is spray deposition using water-based technologies; the resulting porous CNF templates are excellent candidates to infiltrate conductive polymers for functionalization. We used poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), widely applied in organic photovoltaics and electronics, to functionalize the CNF template. We studied the infiltration, resulting structural rearrangement within the thin CNF film of 400 nm thickness, and their behavior under cyclic humidity changes by grazing incidence small-angle neutron scattering. We resolve in situ reversible morphological rearrangements within pristine CNF thin films under cyclic humidification, which might be attributed to voids or coiling. When infiltrating PEDOT:PSS, morphological changes within the film are inhibited due to the polymer completely filling any porous structure within the thin film during cyclic humidification. The CNF/PEDOT:PSS composite obtained by infiltration rather shows a swelling process of the PEDOT:PSS component in the film. This behavior is reversible over at least two humidification cycles. As humidity is present in many device applications and during processing and fabrication of conductive CNF composites, our results help to understand the humidity's nanoscale impact to the meso- or macroscale in a device application.

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Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

3D-printed humidity chamber for neutron scattering on thin films

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The investigation of thin soft matter films with neutrons allows a non-destructive probe with good scattering statistics. It is used in a broad field of scientific interest that studies structures and performance of various soft matter systems such as hydrogels or organic solar cells. However, soft matter samples are very sensitive to humidity and temperature and require well-defined ambient conditions. As such, specialized sample environments are needed which provide stable control over the thermodynamic parameters at the sample position. In the framework of the FlexiProb project, a quickly interchangeable sample environment for experiments at the European spallation source (ESS) is designed. We focus on the design and fabrication of a specialized sample environment for the investigation of thin film samples with grazing incidence small angle scattering (GISANS). Its core is a 3D-printed humidity chamber that offers the necessary control of thermodynamic parameters such as temperature and humidity. The spherical chamber design has well distributed fluidic channels inside its walls, which provide a stable and rapidly adjustable temperature. The control over the atmospheric composition around the sample is realized by a remote-controlled gas-flow array that mixes up to three different humidified or dry air streams. The novel chamber design provides a first step into 3D-printed sample environment for neutron instrumentation.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

The cold neutron imaging beam line ANTARES

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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.

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Presenter: SCHULZ, Michael

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

Incommensurate magnetic systems studied with the three-axis spectrometer MIRA

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Incommensurate magnetic structures like Helimagnons and Skyrmions are currently intensively studied. Due to their large periodicity they often show very low-lying excitations, where most of the interesting physics is taking place below some meV. The cold-neutron three-axis spectrometer MIRA is an instrument optimized for such low-energy excitations at small Q transfers. Its excellent intrinsic resolution makes it ideal for studying incommensurate magnetic systems. Here we will present several examples for the dynamics of such structures, which have been measured with MIRA.

Primary authors: GEORGII, Robert; SKOULATOS, Markos (TUM); BÖNI, Peter (Technische Universität München)

Presenter: GEORGII, Robert

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

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

Thermal effects on nanoscale morphologies and chemical group vibrations of thermoresponsive double hydrophilic block copolymers in aqueous solutions

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Thermoresponsive double hydrophilic block copolymers exhibit great interest as model scaffolds for pharmaceutical applications due to their controlled potential in drug encapsulation and release. A thorough elucidation of the nanostructure of the formed self-assemblies and its evolution at different temperatures is mandatory to provide tailored design guidelines in targeted therapeutics. We present a summary on the investigation of the internal morphology for aqueous self-assembled nanostructures of novel double thermoresponsive PNIPAM-b-poly (oligo ethylene glycol methyl ether acrylate) (PNIPAM-b-POEGA) block copolymers by small angle neutron scattering (SANS). Our findings propose a distinct impact of chain-end groups on self-assembled morphologies, as well as on the interchain/intrachain interactions. The lower critical solution temperature (LCST) of these block copolymer solutions defines a transition crossover from hierarchical morphologies to well-defined nanoscale morphologies at temperatures above the LCST. Our scattering results are complemented by Fourier-Transform Infrared (FTIR) Spectroscopy. The combined FTIR and SANS data reveal that temperature-dependent vibrations of chemical moieties do not necessarily correlate to the analogous structural transitions at the nanoscale. Thereby, our study provides important insights into the morphology related to these thermoresponsive double hydrophilic block copolymer scaffolds for pharmaceutical applications.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

Putative spin-nematic phase in the square lattice compound BaCdVO(PO4)2

Tuesday, December 8, 2020 1:40 PM (25 minutes)

We report neutron-scattering and ac magnetic susceptibility measurements of the two-dimensional spin-1/2 frustrated magnet BaCdVO(PO4)2. At temperatures well below TN≈1K, we show that only 34% of the spin moment orders in an up-up-down-down stripe structure. Dominant magnetic diffuse scattering and comparison to published muon–spin–rotation measurements indicates that the remaining 66% is fluctuating. This demonstrates the presence of strong frustration, associated with competing ferromagnetic and antiferromagnetic interactions, and points to a subtle ordering mechanism driven by magnon interactions. On applying magnetic field, we find that at T=0.1 K the magnetic order vanishes at 3.8 T, whereas magnetic saturation is reached only above 4.5 T. We argue that the putative high-field phase is a realization of the long-sought bond-spin-nematic state.

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Presenter: Dr SKOULATOS, Markos (TUM)

Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

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

Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules, thus providing important complementary information to that gained by X-ray crystallography. At the MLZ the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is dedicated to structure determination of proteins. 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 protein active centre and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behaviour 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. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography.

Primary authors: OSTERMANN, Andreas; SCHRADER, Tobias

Presenter: OSTERMANN, Andreas

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Highly ordered titania films with incorporated germanium nanocrystals annealed in different atmospheres for photoanodes

Wednesday, December 9, 2020 5:30 PM (20 minutes)

Mesoporous titania films with ordered nanostructures show great promise in various applications, e.g. solar cells. To optimize solar cell performance, pre-synthesized crystalline germanium (Ge) nanocrystals around 10 nm are introduced into mesoporous titania films. The influence of different annealing atmosphere (air and argon) on the morphology and properties of the titania/Ge composite films is studied. Resulting surface and inner morphology changes are investigated by scanning electron microscopy and grazing incidence small-angle X-ray scattering (GISAXS), respectively. Elemental composition of the titania/Ge composite films annealed in air and argon atmosphere is compared via X-ray photoelectron spectroscopy. The crystalline and optical properties are observed by X-ray diffraction, transmission electron microscopy and ultraviolet–visible spectroscopy, respectively. Through the incorporation of germanium nanoparticles with varied weight percent and annealing under different atmospheres, the optimized morphology and properties of titania/Ge composite films will be obtained, providing a promising candidate for solar cell photoanodes.

Primary author: LI, Nian

Co-authors: Mr GUO, Renjun (Technische Universität München); HEGER, Julian; SCHAFFRINNA, Roy (Technische Universität München); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: LI, Nian

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

High-resolution powder diffractometer SPODI

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In this contribution we present an overview on specifications, applications and recent developments at high-resolution powder diffractometer SPODI. The presentation includes the various setups and sample environmental devices which are available for in-situ materials characterization. Another key aspect is the illustration of current research areas, supported by statistics on publications. Finally, an outlook for future developments is presented.

Primary authors: HOELZEL, Markus; SENYSHYN, Anatoliy; BARAN, Volodymyr; Mr PFANZELT, Josef (MLZ /TUM); EHRENBERG, Helmut (KIT)

Presenter: HOELZEL, Markus

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Structure Research

Contribution ID: **56** Type: **Invited talk**

Imaging with fast neutrons - improvements in spatial resolution and quantification

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Fast neutron imaging is a technique to investigate large objects where X-rays or thermal neutrons face limitations due to their comparatively low penetration capabilities. Compared to thermal neutrons, where thin scintillators (< 100um) generally provide good detection efficiencies (» 1%) at high spatial resolutions in the 10th of microns range, fast neutrons currently require mm-thick scintillator materials with low detection efficiencies (~ 1%) at spatial resolutions in the mm-range, often blurring important details in radiographs, such as cracks or small inclusions.
Additionally, the predominant interaction mechanism for fast neutrons is via nuclear scattering in mostly forward direction. This furthermore implicates the traditional imaging approach by placing objects very close to the detector surface to reduce geometrical blurring. In collaboration between the Paul Scherrer Institut (PSI), Forschungs-Neutronenquelle (FRMII) Heinz Maier-Leibnitz, Los Alamos National Laboratory and the company RC Tritec, measurements were performed at the FRMII and LANL to characterize the impact of the mentioned challenges and to find a pathway for quantification and standardization of imaging setups at different facilities, as well as for improving resolution and efficiency of the technique in a collaborative effort.
Here we present the results of these measurements, including a break-through in improved spatial resolution by use of a new scintillator concept for fast neutrons.

Primary authors: Dr LEHMANN, Eberhard (PSI); Dr MANNES, David (PSI); Dr STROBL, Markus (PSI); Dr WALFORT, Bernhard (RC Tritec); Dr LOSKO, Adrian (TUM); Dr SCHILLINGER, Burkhard (TUM); Dr SCHULZ, Michael (TUM); Dr VOGEL, Sven (LANL); Mr SCHAPER, Danielle (LANL)

Presenter: Dr LEHMANN, Eberhard (PSI)

Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

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

Stimuli-Responsive Micelles from Amphiphilic Diblock Copolymers

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Stimuli-responsive block copolymers self-assemble in aqueous solution and respond to changes of their environment, rendering them useful as smart nanocarriers for drug delivery and gene therapy. In the present project, we investigate responsive micelles formed by PDMAEMA-***b***-PLMA or PDMAEMA-***b***-PLMA-***b***-POEGMA [1,2]. PDMAEMA is a weak cationic polyelectrolyte and responsive to pH, ionic strength and temperature, whereas PLMA is strongly hydrophobic, enabling the delivery of hydrophobic drugs. POEGMA is permanently water-soluble and improves biocompatibility. Dynamic light scattering on PDMAEMA70-***b***-PLMA39 revealed that, at pD 2.8, self-assembled structures form, whose relatively large size points to vesicle formation. At pD 7.8 and 10.4, additional large aggregates are present up to a certain temperature. Detailed structural information is obtained from small-angle neutron scattering (SANS) at KWS-2 at MLZ, confirming the differences of the micellar structures in acid or alkaline solution.

Primary authors: LI, Yanan (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie); KANG, Jia-Jhen (Technical University of Munich); SKANDALIS, Athanasios (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation); CHRYSOSTOMOU, Varvara (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation); RADULESCU, Aurel (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ); Dr PISPAS, Stergios (Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation); PAPADAKIS, Christine (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie)

Presenter: LI, Yanan (Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

The new Total Reflection High-Energy Positron Diffractometer at NEPOMUC

Wednesday, December 9, 2020 5:40 PM (20 minutes)

It has been shown that Total Reflection High-Energy Positron Diffraction (TRHEPD) is an ideal technique to precisely determine the crystalline structure of the topmost and immediate subsurface layers. Novel materials such as topological insulators or 2D materials can be investigated to determine not only the surface structure, but also the substrate spacing and potential buckling.

We developed a novel TRHEPD apparatus, which is now connected to the high-intensity positron source NEPOMUC at the FRM II. During the first beamtime in spring 2020, it was possible to magnetically guide the positron beam to the experiment, test the electrostatic acceleration up to 15keV and map the direct beam using a micro channel plate (MCP) assembly. We obtained a parallel beam suitable for diffraction with a diameter of less than 4mm. We also tested the optional twofold remoderation device in front of the TRHEPD setup that reduces the beam diameter to about 1mm. These values are in excellent agreement with our simulations. For the next beamtime, we plan to record the first diffraction pattern of a Si(111)-(1x1) hydrogen-terminated surface to benchmark the setup. Recent experimental results will be presented at the meeting.

Primary author: Mr DODENHÖFT, Matthias (Technische Universität München (TUM) Physik Department E21 und Heinz Maier-Leibnitz Zentrum (MLZ) Lichtenbergstr. 1 85748 Garching, Germany)

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

A GISANS study of bio-hybrid films: Influence of pH on spray-coated ß-lactoglobulin:TiO2 film morphology for bio-templated titania nanostructures

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Nanostructured metal oxides such as TiO2 play a major role in hybrid photovoltaics. They can serve as the inorganic charge acceptor of the active layer. For this, a designed structure is of high importance to address different challenges on different length scales. This includes mesoscopic pores for an eased backfilling of the organic donor material and a high interfacial area between donor and acceptor domains, having domain sizes of tens of nanometers for efficient charge carrier separation. A hierarchical morphology of high surface-to-volume ratio is hence beneficial for the device performance. Diblock copolymer directed sol-gel chemistry offers a way to fabricate templated TiO2 films on an industrially relevant scale, e.g. by spray-coating. However, involved organic solvents lead to a restricted potential in environmentally friendly processing. To overcome this issue, we investigate water-based sol-gel templating with the use of biopolymers. The bovine whey protein ß-lactoglobulin is known to form differently structured aggregates by denaturing at different pH values. In combination with a water-based TiO2 precursor, different bio-hybrid film morphologies are obtained by spray-coating. The influence of pH on the film morphology is investigated by bulk and surface-sensitive grazing incidence small-angle neutron scattering (GISANS). The obtained results are complemented by real-space imaging with scanning electron (SEM) and atomic force microscopy (AFM).

Primary author: HEGER, Julian Eliah

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Presenter: HEGER, Julian Eliah

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Spray deposited anisotropic magnetic hybrid thin films containing PS-b-PMMA and strontium hexaferrite magnetic nanoplates

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Spray deposition is employed to fabricate anisotropic ferromagnetic thin films composed of the ultrahigh molecular weight diblock copolymer (DBC) polystyrene-*block*-poly(methyl methacrylate) and strontium hexaferrite nanoplates functionalized with hydrophilic groups. During spray deposition, the kinetics of structure evolution of the hybrid films is monitored in situ with grazing incidence small angle X-ray scattering. A pure polymer film is also deposited as a reference with same conditions. The obtained final hybrid film is then solvent annealed to increase the domain size of the DBC for the incorporation of more nanoplates. Due to the rearrangement of the nanoplates inside the DBC during solvent annealing, an obvious change in the magnetic behavior of the hybrid film is observed via superconducting quantum interference device investigation. After solvent annealing, the hybrid film shows extremely weak magnetic anisotropy. While it exhibits magnetic anisotropy before solvent annealing.

Primary authors: Mr CAO, Wei (TU München, Physik-Department); Ms YIN, Shanshan (TU München, Physik-Department); Ms PLANK, Martina (TU Darmstadt, Ernst-Berl-Institute for Technical and Macromolecular Chemistry); Dr OPEL, Matthias (Walther-Meissner-Institut); Prof. GALLEI, Markus (Saarland University, Organic Macromolecular Chemistry); Dr CHEMEZOV, Andrei (DESY); Mr BRETT, Calvin J. (DESY. KTH Royal Institute of Technology); Dr SCHWARTZKOPF, Matthias (DESY); Prof. ROTH, Stephan V. (DESY. KTH Royal Institute of Technology); Prof. MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department)

Presenter: Mr CAO, Wei (TU München, Physik-Department)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Low-Energy Positron Beam for Near-Surface Doppler-Broadening Spectroscopy

Wednesday, December 9, 2020 5:40 PM (20 minutes)

A new positron beam setup has been put into operation for Doppler-broadening experiments with low energy positrons in order to allow the investigation of surfaces and near-surface defect structures. Positrons provided by a ^{22}Na source are moderated in a 1 μm single crystalline tungsten foil from which they are guided to the sample chamber by longitudinal and transverse magnetic fields. The positrons are accelerated electrostatically by a potential difference applied between moderator and sample. Kinetic energies as low as 1 eV and up to 30 keV are possible. Inside the UHV chamber the positron beam is focused onto the sample by an electrostatic single lens.
Instead of the standard sample holder a heatable one can be mounted.
This setup is intended to complement the positron instrument suite at NEPOMUC and expands capabilities in the field of defect studies at and near the surface. First experimental results on oxides will be presented.

Primary author: MATHES, Lucian

Co-authors: FRANZ, Julian; MITTERREITER, Marc; VOHBURGER, Sebastian; HUGENSCHMIDT, Christoph; BURWITZ, Vassily Vadimovitch

Presenter: MATHES, Lucian

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **62** Type: **Talk**

Self-similar structure and dynamics of polymer rings.

Thursday, December 10, 2020 1:30 PM (15 minutes)

Small Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE) results on very large poly(ethylene-oxide) (PEO) rings in the melt are presented [1,2]. The ring conformation demonstrate a clear signature of the theoretically predicted elementary loops. Their size is in the range of an entanglement strand for linear PEO melts and they are characterized by Gaussian statistics. The ring chain length dependence of the radius of gyration Rg follows rather closely the prediction of decorated ring model [3]. Other than extracted from numerous simulations that are interpreted in terms of a cross over to mass fractal, such a cross over was not observed by SANS. We could also clarify the unique topology driven self-similar ring dynamics and distinguish between different scaling theories. While the dynamics of linear and branched polymers is dominated by the celebrated reptation mechanism, where a polymer creeps out of its topological confinement via its ends, polymer rings featuring no ends cannot undergo reptation but are supposed to perform self-similar dynamics. We present NSE experiments on the initial anomalous center of mass diffusion and the internal dynamics of large polymer rings –a field of broad interest that so far has exclusively been accessed by theory and simulations.

[1] M. Kruteva et al. ACS Macro Lett. 9 (2020) 507–511
[2] M. Kruteva et al. Phys. Rev. Lett., submitted
[3] S. Obukhov et al. EPL 105 (4) (2014) 48005

Primary authors: Dr ALLGAIER, Jürgen (JCNS); Prof. RICHTER, Dieter (JCNS); KRUTEVA, Margarita (JCNS); MONKENBUSCH, Michael (JCNS)

Presenter: KRUTEVA, Margarita (JCNS)

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

Estimation of lithiated cathode loss for cycled 18650-type battery by in situ neutron powder diffraction

Wednesday, December 9, 2020 5:40 PM (20 minutes)

18650-type cells comprising of LiNi0.54Co0.15Mn0.31O2 and LiNi0.87Co0.07Al0.06O2 as cathode and graphite as the anode are cycled at various SoC ranges. Inconsistent capacity fade is found, indicating that the medium SoC range cycling with less capacity loss behaves better than the high and low SoC ranges, while the low SoC range cycling tends to have nonlinear capacity fade. The non-destructive methods, in situ neutron powder diffraction (NPD) at SPODI, is used to obtain detailed structural information about the cathode and anode materials without opening the cell. The crystalline phases in the cell are identified and their lattice parameters and respective weight fractions are calculated. Loss of lithium inventory (LLI) is calculated by the relative weight ratio of LiC6 and LiC12, indicating that LLI is the dominating degradation factor for the inconsistent capacity fade of cells. The lithiated cathode loss is caused by the trapping of lithium in the cathode under the controlled battery cycling voltage window (2.5V - 4.2V), which leads to the mobile lithium and cathode material loss. Lithiated cathode loss is estimated by the observation of cathode unit volume change. The estimated lithiated cathode loss accounts for approximately half of the total LLI. The pulverization of the cathode particles is observed by SEM. The disintegration of the cathode particle causes the contact loss with active material inactivity, which is the main reason for the lithiated cathode loss.

Primary authors: ZHU, Jiangong; KNAPP, Michael (KIT, IAM-ESS); SØRENSEN, Daniel (MLZ); HEERE, Michael; SENYSHYN, Anatoliy; EHRENBERG, Helmut (KIT)

Presenter: ZHU, Jiangong

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Structure Research

Contribution ID: **64** Type: **Talk**

Phonon renormalization explained by electron-momentum dependent electron-phonon coupling

Thursday, December 10, 2020 4:00 PM (15 minutes)

Electron-phonon coupling, i.e., the scattering of lattice vibrations by electrons and vice versa, is a common phenomenon in solids and can lead to emergent ground states such as superconductivity and charge-density wave order. Signatures of strong electron-phonon coupling, e.g. softening and broadening of phonons on cooling, are typically assigned to the presence of nested parts of the Fermi surface or lattice anharmonicity. Here, we unravel a third scenario in the seminal strong-coupling material YNi_2B_2C. The three-dimensional Fermi surface features a large value of the electronic joint density-of-states but only fro a particular value of the electron out-of-plane momentum k_z. Using a combination of inelastic neutron scattering and angle-resolved photoemission spectroscopy analyzed based on *ab-initio* lattice dynamical calculations we show that this peak of the electronic joint density-of-states as function of k_z is likely the origin for the spectacular phonon renormalization in YNi_2B_2C. Thus, our study rationalizes strong phonon anomalies in the absence of both classic, i.e. phonon-momentum dependent nesting and anharmonicity.

Primary authors: Mr KURZHALS, Philipp (Karlsruhe Institute of Technology); Dr KREMER, Geoffrey (University of Fribourg); Dr JAOUEN, Thomas (University of Fribourg); Dr NICHOLSON, Chris (University of Fribourg); Dr HEID, Rolf (Karlsruhe Institute of Technology); Dr NAGEL, Peter (Karlsruhe Institute of Technology); Dr CASTELLAN, John-Paul (Karlsruhe Institute of Technology); Dr IVANOV, Alexander (Institut Laue Langevin); Dr STROCOV, Vladimir (Paul-Scherrer Institut); Prof. MONNEY, Claude (University of Fribourg); Prof. REZNIK, Dmitry (University of Colorado at Boulder); WEBER, Frank (Karlsruhe Institute of Technology)

Presenter: WEBER, Frank (Karlsruhe Institute of Technology)

Session Classification: DN2020: Materials

Track Classification: DN: Materials

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

Fabrication on Plasmonic Nanostructures in Photoelectronic Devices

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Plasmonics include various aspects of surface plasmons, which utilize light-metal interactions. In applications, surface plasmon polaritons (SPPs) and the near field from localized surface plasmon resonances (LSPRs) can be beneficial for light absorption as well as electrical characteristics of photoelectronic devices. The utilization of plasmonic metal nanoparticles (NPs) is frequently proposed as a means to further enhance the light absorption in the broad wavelength range as well as to facilitate charge collection and transport in the photoelectronic devices. Therefore, it is of crucial importance to fabricate suitable plasmonic nanostructures and investigate their fundamentals in photoelectronic devices. Advanced scattering methods such as grazing incidence small/wide-angle x-ray scattering (GISAXS and GIWAXS) were used to study plasmonic structures implemented in photoelectronic devices.

Primary author: Mr GUAN, Tianfu

Co-authors: Dr CHEN, Wei; Mr GUO, Renjun; Mr LIANG, Suzhe; L. WEINDL, Christian; Mrs LI, Nian; Prof. MÜLLER-BUSCHBAUM, Peter

Presenter: Mr GUAN, Tianfu

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **66** Type: **Talk**

Cononsolvency-induced collapse transitions in thermo-responsive block copolymer films

Thursday, December 10, 2020 3:45 PM (15 minutes)

The diblock copolymer PMMA-b-PNIPAM forms micelles in solution that feature a permanently hydrophobic core and a thermo-responsive shell. While a typical shell collapse transition can be induced via a temperature stimulus at the LCST, the PNIPAM block is also sensitive to the composition of the surrounding solvent. Although water and organic cosolvents individually act as good solvents to the PNIPAM chain, mixtures of both act as bad solvent. As a consequence, the transition temperature shifts as a function of the molar fraction of the cosolvent. For PNIPAM, well-known examples of cosolvents include simple alcohols such as methanol or ethanol as well as acetone. We demonstrate that the cononsolvency effect is transferrable from solution to thin film systems. PMMA-b-PNIPAM films swollen in saturated water vapor show a swelling and collapse at the exchange of the surrounding atmosphere to a mixed vapor of water and cosolvent. The film kinetics are investigated with a focus on time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance techniques. In order to differentiate between water and cosolvent distributions along the films'vertical, sequential experiments with deuterated and non-deuterated water and cosolvent are performed. Complementary FTIR measurements reveal the hydration and cosolvent exchange process at the PNIPAM amide and alkyl functional groups.

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

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

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

PMMA-b-PNIPAM thin films display cononsolvency driven response in mixed water-methanol atmospheres

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The diblock copolymer PMMA-b-PNIPAM forms micelles in solution that feature a permanently hydrophobic core and a thermo-responsive shell. While a typical shell collapse transition can be induced via a temperature stimulus at the LCST, the PNIPAM block is also sensitive to the composition of the surrounding solvent. Although water and organic cosolvents individually act as good solvents to the PNIPAM chain, mixtures of both act as bad solvent. As a consequence, the transition temperature shifts as a function of the molar fraction of the cosolvent. For PNIPAM, well-known examples of cosolvents include simple alcohols such as methanol or ethanol as well as acetone. We demonstrate that the cononsolvency effect is transferrable from solution to thin film systems. PMMA-b-PNIPAM films swollen in saturated water vapor show a swelling and collapse at the exchange of the surrounding atmosphere to a mixed vapor of water and cosolvent. The film kinetics are investigated with a focus on time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance techniques. In order to differentiate between water and cosolvent distributions along the films'vertical, sequential experiments with deuterated and non-deuterated water and cosolvent are performed. Complementary FTIR measurements reveal the hydration and cosolvent exchange process at the PNIPAM amide and alkyl functional groups.

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

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Phonon renormalization in $LaCoO_3$

Wednesday, December 9, 2020 5:40 PM (20 minutes)

LaCoO3 features two broad crossovers observed around $T_1 = 100\,\mathrm{K}$ and $T_2 = 200\,\mathrm{K}$. These crossovers are typically associated with the temperature dependent population of excited spin states of the Co^{3+} ion, which evolves upon heating from the low-spin (LS), $S = 0$, to high-spin (HS), $S = 2$, configuration. Since the CoO_6 octahedra expands around the larger HS sites, a static LS-HS order was proposed by Goodenough in the 1960's [1] but was never confirmed experimentally. More recent studies [2,3] propose a dynamic short-range order of alternating LS and HS Co sites. A corresponding dynamic distortion of the crystal lattice mimics closely the Co-O breathing mode. Here, we use inelastic neutron scattering to study the lattice dynamics of $LaCoO_3$ over a wide temperature range, $5\,\mathrm{K} \leq \mathrm{T} \leq 700\,\mathrm{K}$. We find strong phonon renormalization of low- as well as high-energy phonon modes with periodicities corresponding to the proposed superlattice.

[1] P. M. Raccah and J. B. Goodenough, Physical Review 155, 932 (1967).
[2] J. Kuneš and V. Křápek, Physical Review Letters 106, 256401 (2011).
[3] V. Křápek et al., Physical Review B 86, 195104 (2012).

Primary authors: Dr KAUTH, Maximilian (Karlsruhe Institute of Technology); Dr HEID, Rolf (Karlsruhe Institute of Technology); Dr CASTELLAN, John-Paul (Karlsruhe Institute of Technology); PARK, Jitae; Dr MITCHELL, John (Argonne National Laboratory); WEBER, Frank (Karlsruhe Institute of Technology)

Presenter: WEBER, Frank (Karlsruhe Institute of Technology)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Quantum Phenomena

Contribution ID: **69** Type: **Poster**

The Coincidence Doppler-Broadening Spectrometer at NEPOMUC

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Doppler-broadening spectroscopy (DBS) of the 511keV gamma line generated by positron-electron annihilation provides information on lattice defects. It is sensitive to concentrations as low as 1e-7 vacancies per atom. In addition, the chemical surroundings of defects can be analyzed by coincidence DBS (CDBS). The current status and recent improvements of the CDB-Spectrometer at the Neutron-induced Positron Source Munich (NEPOMUC) is presented.
The maximum probing depth of the positron beam is material dependent and varies from hundreds of nm, for heavy metals to a few micrometers in, e.g., Si. Two beam modes are available: standard measurements with a $\approx$ 300 μm (FWHM) beam spot and high resolution measurements with a micro beam with a spatial resolution of 33 μm (FWHM). Measurements may either be conducted as DBS, where the signal at each detector is treated separately, or as CDBS, where the detectors are run as coincidence pairs, greatly improving the signal-to-noise ratio. Currently, three different sample holders are available: i) a piezo x-y stage for precision 2D scanning and hence 3D defect imaging, ii) a heatable sample holder with $T_{max} = 1100$ K for temperature dependent defect spectroscopy, iii) a cryostat with $T_{min} = 40$ K.
The improvements comprise an automated beam optimization system and the increase in the number of detectors combined with an upgrade of the readout electronics.

Primary authors: BURWITZ, Vassily Vadimovitch; MATHES, Lucian; HUGENSCHMIDT, Christoph

Co-authors: VOHBURGER, Sebastian; CHRYSSOS, Leon

Presenter: BURWITZ, Vassily Vadimovitch

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Tracking the formation of MAPbI3 by in situ GIWAXS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Elucidating structure-function relationships in perovskite based materials for photovoltaic and LED application is important to push this material class towards commercialization. Focusing on scaling up methods and working out differences to well established deposition methods, e.g. spin casting, might open up unexpected possibilities for low-cost fabrication.
Slot-die coating is one very promising deposition method for high output production. In this work we investigate the conversion of printed PbI2 on ITO with printed methylammonium iodide (MAI) towards methylammonium lead iodide (MAPbI3) by in situ grazing incidence wide angle X-ray scattering (GIWAXS). Using synchrotron radiation, a time resolution of less than 1 s was achieved and the kinetics of the reaction becomes visible. Time resolved texture evolution during the formation of MAPbI3 shows the connection between preferential orientation of the "precursor" PbI2 thin-film and the final perovskite film, which shows face-on and corner-on orientation (cubic indexing). In contrast, spin-cast MAPbI3 prepared from the same solution and converted with identical parameters shows edge-on orientation. Time resolved deterioration of initially existing solvent-PbI2 complexes is also shown .
The fabrication method and precursor systems have a significant influence on the resulting film morphology, which is highly relevant for optimizing perovskite absorber layers for PV or LED applications.

Primary author: SCHEEL, Manuel (TUM E13)

Co-authors: REB, Lennart (TUM E13); GUO, Renjun (Physics E13, Technical University in Munich); GENSCH, Marc (DESY); SCHWARTZKOPF, Matthias (DESY); ROTH, Stephan (DESY / KTH); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: SCHEEL, Manuel (TUM E13)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **71** Type: **Invited talk**

The hunt for enzyme isoform specific ligand binding: using neutron crystallography to elucidate selective inhibition of carbonic anhydrase by saccharin-based ligands.

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Up-regulation of carbonic anhydrase IX (CA IX) expression is an indicator of cancer metastasis and is associated with poor cancer patient prognosis. As such, CA IX has emerged as an attractive cancer target for diagnosis, cancer staging, imaging, and also treatment. However, due to the high level of sequence conservation between human variants of the enzyme, development of isoform-specific inhibitors has been largely unsuccessful. In this study, a CA IXmimic construct that mimics the CA IX active site while maintaining CA II characteristics that make it amenable to crystallography. The mimic construct is based on CA II but with seven point mutations introduced to match the greater active site region with >96% identity to that of CA IX. The structures of CA IXmimic unbound and in complex with saccharin (SAC) and a saccharin-glucose conjugate (SGC) were determined using joint X-ray and neutron protein crystallography. Previously, SAC and SGC have been shown to display CA isoform inhibitor selectivity in assays but X-ray crystal structures failed to reveal the basis of this selectivity. Joint X-ray and neutron crystallographic studies have shown which active site residues play a role and how solvent displacement and H-bonding reorganization occurs prior to - or upon - SAC and SGC binding. Specifically, these observations highlighted the importance of residues 67 (Asn in CA II, Gln in CA IX) and 130 (Asp in CA II, Arg in CA IX) in selective CA inhibitor targeting.

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Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

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

Water dynamics in a concentrated aqueous solution of perdeuterated poly(N-isopropylacrylamide) across the cloud point

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In aqueous solutions of the thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM), the interaction between water and the polymer changes strongly at the demixing transition. Cooperative dehydration causes the polymer chains to collapse and aggregate. Recent quasi-elastic neutron scattering experiments have shown that the susceptibility spectra of hydration water occur at lower frequencies than those of bulk water and that their relative population decreases abruptly at the cloud point [1,2].
In the present study, we investigate the low frequency water dynamics on a perdeuterated PNIPAM sample in H_2O using the backscattering spectrometer SPHERES at FRM II with an increased energy resolution near the elastic line of ~0.65 μeV (FWHM). Deuteration suppresses incoherent scattering from the polymer. We find that, below the cloud point, the previously observed frequency dependence of the relaxation of the hydration water extends to lower frequencies. Below, but even more strongly above the cloud point, an additional slow process is detected and is tentatively attributed to strongly bound water.

1. M. Philipp, C. M. Papadakis et al., J. Phys. Chem. B 2014, 118, 4253
2. B.-J. Niebuur, C. M. Papadakis et al., Macromolecules 2019, 52, 1942

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

The resonant neutron spin echo spectrometer RESEDA

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The MIEZE (Modulation of Intensity with Zero Effort) technique is in essence a high-resolution spin echo time-of-flight technique. In contrast to classical neutron spin echo, all beam preparation and therefore all spin manipulation is done BEFORE the sample, opening up the possibility of introducing depolarizing conditions at the sample position. Therefore, magnetic or strongly incoherently scattering samples can easily be measured without loss of signal. Furthermore, it is possible to apply large magnetic fields at the sample position, making MIEZE an excellent tool for studying fluctuations at quantum phase transitions as well as other dynamic magnetic phenomena, such as the melting of superconducting vortex lattices. Several highlights of recent results utilizing measurements from RESEDA using the MIEZE technique will be presented.

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Presenter: JOCHUM, Johanna K.

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Magnons in the collinear antiferromagnetic phase of Mn5Si3

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The antiferromagnetic compound Mn5Si3 is an interesting material for applications since it is hosting rich physics, such as the inverse magnetocaloric effect [1] and a large anomalous Hall effect [2]. Despite the intense research activity over the past decades [1-5], many open questions remain regarding the minimal magnetic model Hamiltonian, the role of the spin fluctuations in the magnetically ordered phases and which Mn site is responsible for them. We addressed some of these problems by combining polarized and unpolarized inelastic neutron scattering measurements and density functional theory calculations. We investigated the electronic and magnetic properties of the system and determined the magnetic exchange interactions and the biaxial magnetocrystalline anisotropy in the high temperature collinear antiferromagnetic phase of Mn5Si3. This provided the parameters for a Heisenberg model, from which we computed the spin-wave energies as a function of the external magnetic field applied perpendicular to the preferred axis. Our experimental data and theoretical results are in good agreement with each other.
[1] N. Biniskos et al; Physical Review Letters 120, 257205 (2018).
[2] C. Sürgers et al; Scientific Reports 7, 42982 (2017).
[3] M. Gottschlich et al; Journal of Materials Chemistry 22, 15275 (2012).
[4] P.J. Brown et al; J. Phys.: Condens. Matter. 4, 10025 (1992).
[5] P.J. Brown and J.B. Forsyth; J. Phys.: Condens. Matter. 7, 7619 (1995).

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

Contribution ID: **75** Type: **Poster**

In Operando Neutron Reflectometry Study of SEI Formation on Lithium Metal Anodes Modified with PS-b-PEO Thin Films

Wednesday, December 9, 2020 5:35 PM (25 minutes)

Due to the high theoretical capacity (3860 mAh g-1) and the lowest discharge/charge potential (-3.04 V vs. standard hydrogen electrode) of the lithium metal anode, rechargeable lithium metal batteries have been identified as one of the most advanced energy storage systems, which hold great promise for practical applications. However, lithium metal batteries suffer from serious safety concerns and poor cycling stability, which can be attributed to the uncontrolled growth of lithium dendrites and the unstable formation of the solid electrolyte interface (SEI). Interface property engineering by surface modification of the lithium metal electrode is one of the most promising methods to improve the electrochemical performance of lithium-metal batteries. Using amphiphilic block copolymers to modify the lithium metal anode is regarded as an effective method to enhance its electrochemical performance. Therefore, we are aiming to study the effect of the amphiphilic block copolymer modification and its morphology on the SEI formation and the final electrochemical performance. Due to the sensitivity to light elements in the SEI compounds, neutron reflectometry (NR) is an ideal technique to investigate the layer thickness, roughness, and the layers scattering length density (SLD) of the SEI. By comparing the experiment data, the effect of block copolymer modification layer on the Li metal anode on the formation of SEI can be elucidated clearly.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **76** Type: **Talk**

Membrane stiffness and interaction of lipids with myelin basic protein in native and multiple sclerosis diseased myelin mimetic

Thursday, December 10, 2020 4:30 PM (15 minutes)

A major component of the saltatory nerve signal conduction is the multilamellar myelin membrane around axons. In demyelinating diseases like multiple sclerosis, this membrane is damaged which leads to severe problems in nerve conduction. In literature different values for the lipid composition of healthy myelin sheath and myelin in the condition of experimental autoimmune encephalomyelitis - the standard animal model for multiple sclerosis - have been found. In this work we try to elucidate the interaction mechanism of myelin basic protein - the structural protein responsible for the cohesion of the cytoplasmic leaflets of the myelin sheath - with membranes mimicking both compositions. As samples we use unilamellar vesicles and supported bilayer systems. With neutron and x-ray small angle scattering methods combined with cryo-TEM we can follow the rapid aggregation which leads to a slow process in which different structures are formed depending on the lipid composition. This structural information can be associated with the bending rigidity of the respective membrane measured with Neutron Spin Echo. Neutron reflectometry gives insights on how the interaction mechanism between membrane and protein functions and reveals how modified membranes are destabilized by the protein.

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Session Classification: DN2020: Life Science/ Biology

Track Classification: DN: Life Science/ Biology

Contribution ID: **77** Type: **Poster**

Probing the complex loading-dependent structural changes in ultrahigh drug-loaded polymer micelles by small-angle neutron scattering

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Drug-loaded polymer micelles or nanoparticles are being continuously explored in the fields of drug delivery and nanomedicine. Commonly, a simple core–shell structure is assumed, in which the core incorporates the drug and the corona provides steric shielding, colloidal stability, and prevents protein adsorption. Recently, the interactions of the dissolved drug with the micellar corona have received increasing attention. Here, using small-angle neutron scattering, we provide an in-depth study of the differences in polymer micelle morphology of a small selection of structurally closely related polymer micelles at different loadings with the model compound curcumin. This work supports a previous study using solid-state nuclear magnetic resonance spectroscopy and we confirm that the drug resides predominantly in the core of the micelle at low drug loading. As the drug loading increases, neutron scattering data suggests that an inner shell is formed, which we interpret as the corona also starting to incorporate the drug, whereas the outer shell mainly contains water and the polymer. The presented data clearly shows that a better understanding of the inner morphology and the impact of the hydrophilic block can be important parameters for improved drug loading in polymer micelles as well as provide insights into the structure-property relationship.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

In-situ neutron diffraction studies on micro- and macrostrains in Ni-base superalloys

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Polycrystalline Ni-base superalloys are frequently used materials for high-temperature applications like turbine discs. To get a deep knowledge of the precipitation kinetics during the thermo-mechanical production process and under service conditions, a new testing machine is built at the Research Neutron Source (FRM II) at MLZ in Germany to perform tension and compression loading up to 100 kN at temperatures up to 1200 ℃ in the neutron beam. In this contribution, results on in-situ tensile tests are presented that were performed on bulk samples of polycrystalline Ni-base superalloys at temperatures up to 600 ℃ at the STRESS-SPEC neutron diffractometer. In-situ neutron diffraction enabled to identify the fraction of the existing phases and their lattice parameters depending on mechanical and thermal loading. In particular, it was possible to determine the change in the preferred crystallographic orientation and the defect density in various phases in the elastic and plastic deformation regime.

Primary authors: KUEMMEL, Frank; SOLIS, Cecilia; MUNKE, Johannes; HOFMANN, Michael; GILLES, Ralph

Presenter: KUEMMEL, Frank

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Conformational and Characteristic Modulation of Prothymosin Alpha following the Addition of Guanidinium Chloride investigated with X-ray / Neutron Scattering Techniques

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Prothymosin Alpha (ProTa) is one of the peculiar intrinsically disordered proteins. It is strongly negatively charged and is directly involved in various cellular mechanisms such as chromatin modification. Previous studies on that protein using single molecule techniques revealed structural changes when exposed to a strong denaturant Guanidinium Chloride (GndCl). Additionally, the emergence of internal friction being relevant for protein chain motion has also been observed. Now similarly, it is studied using small angle X-ray scattering (SAXS) and neutron spin echo spectroscopy (NSE). SAXS experiment shows first structural collapse at 1M GndCl and consecutive expansion at higher GndCl concentrations; indicating dual functionality of the denaturant. Additionally, in spite of reaching similar level of expansion, ProTa at 0M and 6M differs in terms of its degree of flexibility. Static quantities such as persistence length and characteristic ratio show enhanced flexibility with increasing GndCl concentration. This is in agreement with dynamic rigidity probed by NSE which also distinguishes between the two species. Moreover, in contrast to the previous study using FCS, NSE also reveals the existence of internal friction within the peptide chain regardless of GndCl concentration. Finally, a comparison with independent studies of different protein in different denaturant at 6M concentration, suggests a potential universality in the behavior of strongly denatured protein.

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Presenter: HARIS, Luman (Forschungszentrum Jülich)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

Contribution ID: **80** Type: **Talk**

Impact of Sulfur on the melt dynamics of glass forming Ti75Ni25–xSx

Tuesday, December 8, 2020 3:25 PM (25 minutes)

Bulk metallic glasses combine a spectrum of favorable mechanical and chemical properties. Especially Titanium-based bulk metallic glasses are demanded for lightweight construction and for medical devices. However, the presence of toxic Beryllium and the limited casting thickness restricts the production of Titanium-based bulk metallic glasses. Recently, Sulfur was recognized as alloying element for bulk metallic glass production. In Ti75Ni25 the substitution of Nickel by Sulfur leads to bulk metallic glass formation for 8 at.% Sulfur.
In order to identify the origin of the enhanced glass forming ability, we examined the melt dynamics of Ti75Ni25-xSx (x = 0, 5, 8) on different length scales [1]. The mean Ti/Ni self-diffusion coefficients were probed by quasielastic neutron scattering on the time-of-flight-spectrometer TOFTOF. Since Titanium-based melts are highly reactive, we applied containerless processing techniques to perform our experiments. We observe a decrease of melt dynamics for both viscosity and self-diffusion upon Sulfur addition. This is accompanied by a decrease of the melt packing fraction. Neither a reduction of the liquidus temperature nor a dense melt packing can explain the enhanced glass forming ability. Apparently, chemical interactions that lead to the development of a complex melt structure are involved.
[1] J. Wilden, F. Yang, D. Holland-Moritz, S. Szabó, W. Lohstroh, B. Bochtler, R. Busch, A. Meyer (2020) Applied Physics Letters, 117(1), 013702.

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Presenter: WILDEN, Johanna

Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

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

NICOS - Tipps and tricks

Wednesday, December 9, 2020 3:00 PM (3 hours)

NICOS is the standard user interface for the instrument control at the MLZ instruments. Because of the success and the user acceptance the ESS made the decision to used it as well for their instrument control. The SINQ at the PSI was also looking for a new instrument control software and found NICOS.

The webinar is splitted into two sections, a presentation about NICOS with the following topics:

- Introduction into NICOS
- Overview about the newest developments since the user meeting in 2019
- NICOS at SINQ
- New graphical user interface at ESS

and an interactive presentation of NICOS to show some tips and tricks for the users

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Session Classification: MLZ Users 2020 - Webinar NICOS

Track Classification: DN: Digitalization and Machine Learning

Contribution ID: **82** Type: **Talk**

Epsilon - german time-of-flight high resolution neutron diffractometer at the high flux pulsed reactor IBR-2: current status and scientific applications

Thursday, December 10, 2020 2:15 PM (15 minutes)

The TOF diffractometer Epsilon at the beamline 7a of the IBR-2 reactor is dedicated to the high resolution measurements of applied and residual strains of geological samples and functional materials.
A four-axis goniometer permits a rotation around one axis and translation in 3 mutual perpendicular directions. It allows us to measure a strain profile of six independent component of strain tensor. Last years Epsilon had been equipped by variety of dedicated sample environment:
- uniaxial pressure device with possibility of sample rotation under external load with maximal pressure up to 150 MPa for operando measurements;
- an acoustic emission system;
- a laser extensometer for macroscopic deformation measurements of the sample with a resolution of 0.5 μm,
- a triaxial pressure device for operando stress measurements, which allows us in situ determination of Poisson ratio, the bulk modulus and Biot-Willis coefficient.
Epsilon is perfect fitted to the geological application and material sciences, the sample environment is unique and has no analogy through the neutron spectrometers in the world.

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Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

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

In-situ high temperature precipitation study in new alloy VDM 780 using SANS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The new Ni-based superalloy VDM 780, developed for high temperature applications that require good mechanical properties (as gas turbines), shows the presence of only γ'hardening precipitates. The absence of the instable γ"hardening phase, which transforms into δ phase at 650 ℃ resulting in a loss of creep resistance, will allow its use at higher operation temperatures. Due to the direct industrial application of this material, a thorough study of the precipitation process under various heat treatments in this alloy will be fundamental for further improvement of the material.
The precipitation behavior of the VDM 780 Ni-base superalloy was investigated by small angle neutron scattering (SANS) at high temperature. Atom probe tomography (APT) measurements were performed in order to obtain the real composition of the matrix and the precipitates that will allow the calculation of the scattering contrast between them. Two different samples with different heat treatment were used in order to obtain materials at different precipitation steps. SANS allowed to monitor the formation of nano-precipitates and their evolution with temperature. It was found that after the first precipitation step at 720 ℃, the second precipitation step at 620 ℃ produces almost no new precipitates. A sample in a final precipitation state measured at the expected operation temperature of 750 ℃ shows its stability with almost no precipitate growth.

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Presenter: SOLIS, Cecilia

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Utilizing very low flux nuclear reactors for neutron imaging

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In order to provide a basic platform for training and first contact research in the field of neutron science, very low flux facilities represent a sufficient starting point. The training and research reactor (**AKR-2**) with a maximum continuous power of two Watts can be categorized as such a facility. In the course of the last two years, the experimental field of the AKR-2 has been extended by a thermal neutron imaging radiography system (**TRAPY**). Currently, this setup utilizes thermal neutrons with a LiF/ZnS(Ag) scintillator, with the prospect to be able to switch to the fast neutron spectrum in a later setup.

Split in two parts, we first introduce the AKR-2 and the boundary conditions, it provides and continue with first achievements in building and characterizing the imaging setup. So far, the characterization has been made through an L/D study. This study builds upon a previous investigation with a less advanced imaging system (DELCam) and is intended to demonstrate the limits in neutron imaging at AKR-2. A two-way cadmium knife-edge with integrated reproduction scale has been used for the slanted edge method in order to estimate the edge response sufficiently. Additionally, first measurement examples are introduced. It is therefore proposed that experiments not ranked sufficiently high enough for the limited beam time at high flux facilities, but with their experimental needs fulfilled by the AKR-2, can be conducted at our facility.

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Presenter: HÜBSCHER, Rico (TU Dresden)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Cryo-TEM –A Complementary Technique for Neutron Scattering

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The neutron instrumentation at the MLZ, in particular Small Angle Neutron Scattering (SANS), reflectometry and macromolecular crystallography allow to investigate structures in the range from one up to several hundred nm in reciprocal space with high statistical accuracy.
In soft matter and biology the neutron contrast between hydrogen and deuterium is used to gain deep and quantitative insights about the shape and interactions of the objects forming the investigated structure.
Transmission electron microscopy may yield real space pictures 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 investigation on soft matter investigation Both techniques allow to detect structural changes occurring in the relatively large scale structures on the nano-scale.

In order to provide our users the possibility to complete their neutron scattering data, a Cryogenic transmission electron microscope (Cryo-TEM) is available at the Jülich Center for Neutron Sciences at MLZ in the JCNS building.

The instrument as well as the extended suite of preparation equipment will be described and several examples of research investigation in soft matter, particularly nanocomposites, fuel cells, microemulsion, liposomes and polymer self-assembly will be presented.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Understanding mechanical behaviour of Nb3Sn superconducting magnet coils by combined neutron diffraction and macroscopic stress strain measurements

Tuesday, December 8, 2020 3:00 PM (25 minutes)

Reliable mechanical materials data are required for predicting the strain and stress state evolution during assembly, thermal cycling and powering of superconducting magnets. The ingredients for thermomechanical modelling of linear elastic and isotropic magnet materials behaviour are often available. However, taking into account anisotropic mechanical properties, the yielding and flowing of fully annealed Cu, the brittleness of Nb3Sn, and the non-linear and irreversible thermal expansion of the Nb3Sn conductor during reaction heat treatment is particularly challenging. The Nb3Sn conductor block Young's modulus anisotropy and mechanical behaviour are explained based on in-situ neutron diffraction loading strain measurements at the MLZ Stress-Spec diffractometer. It is shown that the conductor block behaves like a fibre reinforced composite, with iso-strain and iso-stress in the conductor constituents under axial and transverse loading, respectively. The potential of different coil characterisation methods, notably digital image analysis and indentation hardness maps in metallographic coil cross sections, and residual strain mapping of collared coil assemblies by neutron diffraction, are compared.

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Presenter: SCHEUERLEIN, Christian (CERN)

Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

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

Advances in neutron and gamma imaging of lead acid batteries

Tuesday, December 8, 2020 3:50 PM (25 minutes)

Nowadays, lead acid batteries still offer a reliable and cost-effective solution compared to lithium-ion batteries, which can be adapted to different types of energy storage applications. After more than 150 years of use, the energy density of these batteries still presents substantial room for improvement. Our research group is monitoring the processes, which occur inside lead acid batteries (ad hoc manufactured small and commercial batteries) in an operando manner. To study their behaviour, we have used thermal and fission neutrons, as well as gamma radiation to perform both radiography and tomography of lead acid batteries with the goal of better understanding their function and subsequently improving their electrochemical efficiency. The type of radiation used can resolve different information. For example, thermal neutron radiography shows that electrolyte stratification is difficult to detect, due the neutron transmission not appreciably changing in the working concentration range of the electrolyte. However, by focusing on the electrodes, evidence for structural and electrochemical evolution in the active materials can be detected based on compositional change. Here, we present a summary of the recent advances we have obtained thus far from experiments performed at DINGO (OPAL reactor, Sydney) and NECTAR (FRM-II reactor, Munich).

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Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **88** Type: **Poster**

The Robot Positioning System at the Materials Science Diffractometer STRESS-SPEC

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The diffractometer STRESS-SPEC is optimised for fast strain mapping and pole figure measurements. Our group was the first to pioneer the usage of industrial robots for sample handling at neutron diffractometers. However, the current robot is limited in its use due to insufficient absolute positioning accuracy of up to ± 0.5 mm. 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 mm^3 –is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. Therefore, the original robot setup at the neutron diffractometer STRESS-SPEC is currently being upgraded to a high accuracy positioning/metrology system. We will present the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 µm or better during strain measurements the sample position will be tracked by an optical metrology system and it is going to be actively corrected. The additional use of radial collimators creates more space in the sample environment and enhance the residual stress analysis capabilities for large complex parts. Finally, a newly designed laser furnace can be mounted at the robot flange to conduct texture measurements at elevated temperatures of up to 1300 ℃. A brief overview of the STRESS-SPEC instrument and its capabilities as well as first commissioning experiments using the new setup will be given

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Non-destructive quantification of lithium and electrolyte losses in Li-ion batteries using neutron powder diffraction

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Lithium-ion batteries lose part of their capacity while they are cycled. This loss is due to various side effects like formation of the solid-electrolyte-interface (SEI), loss of active lithium, etc. The rates of side effects are spatially non-uniformly distributed, due to heterogeneously distributed parameters like temperature and current density. The loss of active lithium can be related to the formation of the SEI, whereas the role of the electrolyte in the SEI formation and its correlation to lithium losses remains not fully clear so far.
Aim of the current study is a non-destructive quantification of lithium and electrolyte, their spatial distributions throughout the cell and concentration changes vs. cell fatigue. High-resolution neutron diffraction independently reveals a direct correlation between losses of active lithium in the graphite anode and these of liquid electrolyte. A non-uniform character of the losses is probed by spatially resolved neutron powder diffraction, thereby displaying the non-trivial character of active lithium/electrolyte losses and complex dynamic of the capacity fading.

Primary author: PETZ, Dominik

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Presenter: PETZ, Dominik

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Evolution of the structure and dynamics of bovine serum albumin induced by thermal denaturation

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Studying thermal protein denaturing provides valuable information on structural and dynamic aspects related to protein function. Here, we use small-angle and quasielastic neutron scattering (SANS and QENS) to shed light on the denaturing of bovine serum albumin (BSA) in the presence and absence of NaCl.

SANS reveals the temperature-dependent formation of a crosslinked BSA network. The sensitivity to NaCl-mediated protein charge screening is furthermore shown to decrease with increasing BSA concentration. A comparison of the dynamical signal from ratios of inelastic and elastic fixed-window scans (FWS) with the dynamical confinement obtained from the apparent mean-squared displacement [1] suggests that the signatures of denaturation observed on nanosecond time scales are dominated by temperature-induced changes of the dynamics. Changes of the local confinement, on the other hand, only contribute weakly. After denaturation, the dynamics is slowed down in the presence of NaCl, while the stability and dynamics of the native solution do not appear to be affected by salt.

Our approach offers a framework for a comprehensive, multi-method characterisation of thermal protein denaturing [2].

[1] Hennig *et al.*, Soft Matter **(8)**, 2012, 1628-1633.

[2] Matsarskaia *et al.*, PCCP, 2020, Accepted Manuscript. DOI: 10.1039/D0CP01857K

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

Wearable smart skin based on triboelectric nanogenerator and CdSe/CdS quantum rods for pressure and tensile sensing

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Over the past few years, wearable smart skin is one of the hottest research topics attracting worldwide attention. Since the birth of the triboelectric nanogenerator (TENG), which is originating from Maxwell's displacement current, the vertical pressure sensor function can be achieved easily without any external power supplies. However, to mimic human skin better, more functions need to be added into one simple device, especially the basic lateral tensile sensing ability.
In this work, we fabricate a new type of wearable smart skin based on TENG and luminescent effect for both vertical pressure and lateral tensile sensing. Polydimethylsiloxane (PDMS) based single-electrode mode TENG part gives the vertical pressure sensing ability to the whole device. In addition, CdSe/CdS quantum rods (QRs) are introduced into the device as a luminescent layer for lateral tensile sensing. Small angle neutron scattering (SANS) is used to investigate the CdSe/CdS QRs alignment in PDMS thick film under different tensile degrees (from 0% to 100%).

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

The zero step for degrading perovskite solar cells: What atmosphere should we choose?

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached the champion value of 25.2 %, making this technique competitive with commercial silicon solar cells. Despite such advantages, the application of PSCs is currently limited by combining high performance and operational stability, because PCE of PSCs can degrade due to the presence of temperature, light, humidity, and oxygen. So far, the degradation research on PSCs is carried out without having an established standard protocol. Therefore, it is necessary to establish a standard protocol for the long-term degradation of PSCs. In this respect, we investigate degradation processes of PSCs under both, AM 1.5G and different atmosphere conditions with in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small-angle X-ray scattering (GISAXS). With these approaches, we can follow the evolution of characteristic structures and of the inner morphology under the respective operational conditions. After understanding the degradation mechanisms upon different atmospheres (nitrogen and vacuum), we can suggest a reasonable atmosphere, which enters the protocol for the standard aging routine to guide future industrial development.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Inward shift in the spin wave dispersion of a stripe discommensurated Pr-based 214-nickelate

Tuesday, December 8, 2020 3:00 PM (25 minutes)

Magnetic excitations in the spin-stripe phases of *La*-based *214*-nickelates have been vigorously explored using INS for almost last three decades and still have remained an exciting research field, especially to understand their differences yet of their structural similarities with high-T_c *214*-cuprates. In view of the reported two-dimensional antiferromagnetic nature, out-of-plane magnetic excitations are generally not expected in *214*-nickelates. From the INS measurements of magnetic excitations in a stripe discommensurated $Pr_{3/2}Sr_{1/2}NiO_4$ with magnetic incommensurability $\epsilon = 0.4$, here we present very compelling evidence for a sizable out-of-plane interaction ($\sim$2.2 meV) which was crucial to explain the observed shift of the spin wave dispersions towards the magnetic zone centers.

Reference: A. Maity, R. Dutta, and W. Paulus, Phys. Rev. Lett. 124, 147202 (2020).

Primary author: MAITY, Avishek

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Presenter: MAITY, Avishek

Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

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

Translocation of non-ionic synthetic polymers through lipid membranes

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Polymers with balanced hydrophilicity can passively translocate through biological membranes without damaging them. In the case of synthetic polymers there are only few reports of translocation using charged polymers. For non-charged polymers translocation phenomena were predicted theoretically but not verified experimentally. Especially these polymers are expected to show weak interactions with bio membranes and are interesting candidates for drug delivery applications.
We have synthesized such balanced amphiphilic polymers which contain alternating low MW hydrophobic and hydrophilic units. We studied translocation properties of the polymers using Pulsed Field Gradient (PFG) NMR and their interactions with lipid membranes using Neutron Reflectometry (NR) and Small Angle Neutron Scattering (SANS). The PFG NMR results show a strong dependence of the translocation rate on polymer molecular weight and hydrophobic block length. The first NR and SANS measurements show that the polymers are partially solubilized in the hydrocarbon part of the bilayer, and the effect is more prominent for less hydrophilic but still water soluble polymers.

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Presenter: KOSTYURINA, Ekaterina

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **95** Type: **Talk**

Perspectives for accelerator based neutron sources - The HBS project

Thursday, December 10, 2020 3:30 PM (15 minutes)

Neutrons can be produced by fission in nuclear reactors, spallation using high-power proton accelerators, and nuclear capture reactions with low-energy proton accelerators. While the first two techniques are used very successfully in Europe, the later option only recently gained greater interest. Using high current low energy proton beams bombarding a metal target a neutron flux comparable with current neutron sources is accessible.
In the HBS project a scalable accelerator driven neutron source optimized for scattering and neutron analytics is developed. The whole chain ranging from the accelerator to the target / moderator / shielding assembly and the neutron optics is optimized to the needs of the neutron experiments. This approach makes the HBS very efficient enabling competitive neutron fluxes at sample position equivalant or better to existing ones. Due to the scalability in accelerator power the source can vary from a low power pulsed neutron source with an average power at the target of a few kW to a high performance neutron source with ~100 kW average power serving as a full-fledged national neutron source.
The baseline specification of the HBS is a high current low energy proton accelerator to drive a 100 kW neutron source serving up to 3 independent target stations with up to 6 individual instruments at each station for experiments. We will describe the current status of the project and its perspective within the European landscape of neutron sources.

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Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

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

SPUTTER DEPOSITION OF SILVER ON NANOSTRUCTURED PMMA-b-P3HT COPOLYMER THIN FILMS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Nanostructured polymer-metal-composite films demonstrate great perspectives for optoelectronic applications, e.g. as sensors [1] or organic photovoltaics (OPV) [2]. To enhance properties of such devices the metal cluster self-assembly process needs to be understood [3, 4]. We correlate the emerging nanoscale morphologies with electronic properties and quantify the difference in silver growth, comparing the diblock copolymer template with its corresponding homopolymer thin film counterparts [5]. Hence, we are able to determine the influence of the respective polymer blocks and to observe substrate effects on silver cluster percolation threshold [5], which affects the insulator-to-metal transition (IMT). In this contribution, we investigate the silver cluster morphology during the growth on a PMMA-b-P3HT block copolymer template. Such block copolymer templates are used as to install tailor nanostructures in OPV, as it contains one p-type organic semiconductor (P3HT) [2]. We applied with grazing incidence small-angle X-ray scattering (GISAXS) to observe the cluster formation, as well as the crystallinity of the metal film formation with grazing incidence wide-angle X-ray scattering (GIWAXS) in situ during sputter deposition. Our study reveals the selective wetting of silver on one of the polymer blocks and the influence of the template on the percolation behavior of the silver layer, which is measured with resistivity measurements during the sputter deposition.

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Presenter: GENSCH, Marc (DESY/TUM)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **97** Type: **Talk**

Neutron Larmor diffraction on nickelate powder samples

Tuesday, December 8, 2020 5:10 PM (25 minutes)

Recently, the discovery of superconductivity in the Sr-doped nickelates $RNiO_2$ (R = Pr, Nd) has attracted widespread attention. The synthesis of the RNiO2 compounds has been achieved by topotactic reduction of the non-superconducting perovskite phase $RNiO_3$, removing oxygen from the crystal lattice in a controlled fashion. Remarkably, new electronic and magnetic phases can also occur in oxygen vacant phases $RNiO_{3-x}$ with intermediate oxygen content 0 < x < 1. For instance, while $LaNiO_3$ remains paramagnetic down to lowest temperatures, long-range antiferromagnetic order emerges in $LaNiO_{2.5}$. However, it has not been clarified yet whether the new electronic and magnetic phases are accompanied by structural phase transitions. Hence, we aim to use the highly sensitive Neutron Larmor diffraction (LD) technique to investigate structural changes that possibly coincide with the electronic and magnetic transitions emerging in oxygen-deficient phases of $RNiO_{3-x}$. As a first step, we report here that LD is capable of detecting the known subtle structural phase transition in $PrNiO_3$ at 120 K, while no transitions were detected in the $LaNiO_3$ sample at low temperatures. Furthermore, a newly introduced analysis technique for LD data allows us to account for resolution effects that originate from small angle scattering from powder samples.

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Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

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

A new high resolution detector system at ANTARES

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The water management in polymer electrolyte membrane fuel cells (PEMFCs) has been studied extensively with neutron imaging. In contrast, for anionic electrolyte membrane fuel cells (AEMFCs), which provide a high economic potential based on the fact that no noble metal catalysers need to be employed, very few studies of water management exist to date.
A main limitation of investigating the water transport in the area of the membrane is the limited spatial resolution of neutron imaging detectors. Several approaches have been made to improve the spatial resolution below the 10µm regime. In this poster we present a novel detector concept which is currently being developed for the ANTARES beam line at FRM II which will be based on the detection of single neutron events and will employ a centroiding technique to increase the spatial resolution down to 1µm.
This project is funded by the BMBF in the framework of ErUM-Pro under the grant number 05K19WO2.

Primary authors: HAN, Yiyong (Heinz Maier-Leibnitz Zentrum); JACOT-GUILLARMOD, Mathieu (Heinz Maier-Leibnitz Zentrum); VEH, Philipp (IMTEK, Universität Freiburg); VIERRATH, Severin (IMTEK, Universität Freiburg); BREITWIESER, Mathias (IMTEK, Universität Freiburg); SCHULZ, Michael

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

High-resolution spectroscopy and diffraction at TRISP

Wednesday, December 9, 2020 5:40 PM (20 minutes)

We present the capabilities of TRISP both for high-resolution spectroscopy and diffraction and show typical experimental examples. TRISP is a thermal three axis spectrometer incorporating the resonant spin-echo technique. Typical applications include the measurement of linewidths of phonons and spin excitations in an energy range 0.5-50meV, and the energy width of quasi-elastic scattering, originating, for example, from critical magnetic fluctuations. Neutron Larmor diffraction (LD) is a high-resolution technique which permits the measurement of lattice spacings d_{hkl} and their distribution Δd_{hkl}. The latter arises, for example, from micro-strains, magnetostriction, structural and magnetic domains, or from a small splitting of Bragg peaks, resulting from distortions of the crystal lattice. The resolution of Larmor diffraction at TRISP is 10^{-6} (relative) for the lattice spacing and one order of magnitude less for the distribution width.

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Presenter: Dr KELLER THOMAS (MPI outstation at the FRM II)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Effect of the protein size on the diffusion of proteins in a cell-like environment - first results from BATS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The investigation of protein diffusion is essential for a comprehensive understanding of living cells.
Recently, the volume fraction dependence of the short-time center-of-mass self-diffusion of immunoglobulin (IgG) in naturally crowded environments has been reported. A remarkable agreement between simulations and experiment explained the agreement between the volume fraction dependence of pure IgG solutions and the naturally crowded samples [1]. The simulations revealed that this agreement is due to the comparable size of the IgG and the averaged size of the cellular lysate serving as crowding agent.

New neutron backscattering measurements with the BATS option of IN16B [2,3] allowed to investigate differently sized proteins in the presence of lysate. Given the increased energy range of BATS maintaining the good energy resolution, it is possible to separate the global diffusion from the internal diffusion. A dependence on the protein size of the diffusion in the presence of deuterated lysate functioning as a crowder has been observed. Global fits, taking the q and energy transfers into account, reveal different hierarchies of the internal diffusion. The comparison with the pure protein solutions at the same volume fractions allowed us to investigate the effects of lysate on the internal diffusion and thus, offer significant insights into the protein properties.

[1] M. Grimaldo et al, JPCL, 2019
[2] C. Beck et al, Physica B, 2019
[3] M. Appel et al, Sci. Rep., 2018

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

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

New analysis frameworks for the analysis of inelastic measurements from neutron backscattering spectrometers

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Recent developments in the instrument design of neutron backscattering spectrometers allow to measure the total scattering function $S(q, \omega)$ with quasi-continous energy transfers but also with specific energy transfers - so called elastic fixed window scans (E/IFWS)- with a high energy resolution. While several models have been developed for the analysis of EFWS [1], there are only few approaches to analyze IFWS.

By reducing the number of energy transfers observed, the corresponding measuring time can be significantly reduced, allowing to investigate samples as a function of control parameters such as temperature-, pressure- or time-dependent samples.

In this contribution, several different approaches are presented to analyze the I/EFWS. This includes the combination of several IFWS as "sparse QENS" [2] , the extraction of generalized mean squared displacements [3] as well as the combination of EFWS and IFWS to extract global diffusion of dissolved proteins [4,5].

The different methods will be analyzed for their suitability for different neutron spectrometers taking into account their resolutions, energy transfers and momentum transfers. Results from modeled data of complex dynamics will be compared to measurements from IN16b (ILL).

[1] D. Zeller, J. Chem. Phys. 2018

[2] K. Pounot, JPCL, 2020

[3] Roosen-Runge et al, EPJ Web of Conf. 2015

[4] O. Matsarskaia et al, PCCP, 2020

[5] C. Beck, PhD Thesis, Univ. Tübingen, 2020

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Short-Time Self-Diffusion of Salt- and Temperature-Dependent Protein Clusters

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Salt-induced charges in aqueous suspensions of proteins can give rise to complex phase diagrams including homogeneous solutions, large aggregates, and reentrant dissolution regimes. Moreover, depending on the temperature, a liquid-liquid phase separation may occur within the aggregation regime. Here, we systematically explore the phase diagram of the globular protein BSA via its dynamics as a function of temperature T and protein concentration c_p as well as of the concentrations c_s of trivalent salts YCl_3 and $LaCl_3$. By employing incoherent neutron backscattering spectroscopy at BASIS (SNS) with energy transfers up to 100 μeV, we unambiguously access the global and internal short-time self-diffusion of the protein clusters depending on c_p, c_s and T. We determine the cluster size in terms of effective hydrodynamic radii as manifested by the cluster center-of-mass diffusion coefficients D. For both salts, we find a simple functional form $D(c_p, c_s, T)$ in the parameter range explored. The master-curve observed previously [1] can be confirmed also for different temperatures and different salts. The salt- specific calculated binding probabilities and inter-particle attraction strengths, based on the short-time microscopic diffusive properties, increase with salt concentration and temperature in the regimes investigated and can be linked to the macroscopic behavior and to microscopy data.

[1] M. Grimaldo et al. J. Phys. Chem. Lett. 6 (2015)

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Presenter: SEYDEL, Tilo (Institut Max von Laue - Paul Langevin)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

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

Following the diffusive processes during a non-classical protein crystallization via neutron spectroscopy

Thursday, December 10, 2020 4:45 PM (15 minutes)

Following dynamics *during* kinetically changing samples is a major challenge. With recent developments of analysis frameworks, accessing the short-time self-diffusive properties of protein solutions by measuring specific energy transfers (FWS) via neutron backscattering, kinetically changing samples can be investigated. More detailed information (internal dynamics and immobile fraction of the proteins) can be extracted from full QENS spectra obtained with a floating average with a lower kinetic time resolution. The immobile fraction, determined by multi-dimensional fits, can be assigned to proteins in a gel-like state or in crystals [1].
Here, we discuss the results of a study performed *during* crystallization. $CdCl_2$ induces a non-classical crystallization process [2,3] of β-lactoglobulin (BLG) with a metastable intermediate phase. We investigated the short-time collective and self-diffusion of BLG by neutron spin-echo (IN11), FWS and QENS (IN16b), respectively, of the crystallization process for different sample conditions. Combining the different results, a consistent picture of the process can be drawn, which differs significantly from classical BLG crystallization induced by $ZnCl_2$ [1]. This implies a strong influence of seemingly subtle cation-specific effects on protein crystallization.
[1] C. Beck, et al., Cryst. Growth Des. 2019
[2] A. Sauter, et al., J. Am. Chem. Soc. 2015
[3] A. Sauter, et.al., Faraday Discuss. 2015

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Presenter: BECK, Christian (Institut Laue Langevin)

Session Classification: DN2020: Life Science/ Biology

Track Classification: DN: Life Science/ Biology

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

MIASANS at the longitudinal resonant spin echo spectrometer RESEDA

Tuesday, December 8, 2020 5:10 PM (25 minutes)

The RESEDA (Resonant Spin-Echo for Diverse Applications) instrument has been optimized for the measurement 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 two precisely tuned radio-frequency (RF) flippers prepare the neutron beam such that it yields a signal of time-varying neutron intensity oscillations. 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). Currently a project is underway to optimize the MIEZE spectrometer for the requirements of small-angle neutron scattering (MIASANS), a versatile combination of the spatial and dynamical resolving power of both techniques. These upgrades include (i) installing new superconducting solenoids as part of the RF flippers to significantly extend the dynamic range (ii) design and installation of modular options for both reflecting guides and evacuated flight paths with absorbing walls for background reduction (iii) installation of a new detector on a translation stage within a vacuum vessel for flexibility in selecting both angular coverage and resolution. Current progress on each of these components will be presented.

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

Presenter: LEINER, Jonathan (Technical University of Munich)

Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

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

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Infrared spectroscopy serves as local probe reporting on specific vibrations in some side chains which are spectrally distant from the complicated infrared spectrum of a protein in solution. But it can also serve as a global probe using the coupling of the amide I or amide II vibrations of the protein backbone. Here, infrared spectroscopy can give information on the fold of the protein and also 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 protein in solution. Both techniques prefer heavy, deuterated water over normal water. Pioneering work has been performed on the combination of SANS and IR spectroscopy using FTIR spectrometers by Prof. Kaneko and coworkers [1].
In the framework of a BMBF-funded project, we would like to explore the capabilities of quantum cascade laser for this combination of methods. Their advantage is superior beam characteristics and spectral density over the glow bar infrared light sources of the FTIR spectrometer. Their disadvantage is the more complicated mode of operation and the limited spectral width they can cover. This contribution will focus on showing conceptual design considerations and first characterizations of potential samples, since the project just started recently (May 2020).
[1] Kaneko et al, Development of a Simultaneous SANS/FTIR Measuring System, Chemistry Letters, 2015, 44, 497-499

Primary author: Dr DADFAR, Seyed Mohammad Mahdi

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Presenter: Dr SCHRADER, Tobias

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

Progress of the MEPHISTO beamline

Wednesday, December 9, 2020 2:50 PM (20 minutes)

The author will present the ongoing process of the beamline MEPHISTO. The upcoming site acceptance test of the experiment PERC including a new Helium liquefier for the super conducting magnet and a temporary setup of the auxiliary components in the neutron guide hall east will be presented. An outlook will be given to the final installation of the auxiliary components on a new attic on the east hall.

Primary author: Dr KLENKE, Jens (FRM II)

Presenter: Dr KLENKE, Jens (FRM II)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Nuclear, Particle, and Astrophysics

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

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Mesoporous Fe2O3 thin films with large area homogeneity demonstrate tremendous application potential in photovoltaic industry, lithium ion batteies, gas or magnetic sensors. In the present work, the synthesis of morphology-controlled Fe2O3 thin films is realized with the polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) diblock copolymer assissted sol-gel chemistry. The effect of the solvent category and polymer-to-FeCl3 ratio is systematicaly investigated during the sol-gel synthesis process. For both DMF and 1,4-dioxane solvent symtem, nanosluster structures are obtained with low PS-b-P4VP concentration, which is supposed to be the result of the weak phase seperation property and thereby the weak template effect of the block polymer. When the concentration of the PS-b-P4VP reaches the critical point of micellization, spherical and wormlike porous structures can be specifically formed in the DMF and 1,4-dioxane solvent system, respectively. The further increase of the polymer-to-FeCl3 ratio lead to the enlargement of the spherical pore size in the DMF system and the shrink of center-to-center distance of the worm like structure in the 1,4-dioxane system.

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

Presenter: YIN, Shanshan

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Chemical analysis with neutrons at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

MLZ offers several instruments for chemical analysis. Prompt Gamma Activation Analysis (PGAA) is located in the neutron guide hall, and uses the strongest cold neutron beam of the world. PGAA is based on radiative neutron capture, and is used for the determination of major and minor components, and several trace elements in the samples non-destructively. The method proved to be unique in the determination of light elements, especially H and B. Many trace elements can be analyzed with much higher sensitivities when using the in-beam activation analysis option.
The same beam is used for Neutron Depth Profiling (NDP), where the concentration profile of certain elements (B, Li) can be determined from the energy loss of neutron induced charged particles. This method has been successfully used in lithium-battery research.
When irradiating the samples in high-flux channels in the reactor, Neutron Activation Analysis (NAA) offers detection limits on the ppb-ppt level for many trace elements. This method has been integrated in our analytical arsenal recently, and has been used for the characterization of meteorites and archaeological objects.
Fast neutrons also generate characteristic gamma radiation, which can be used for the analysis of nearly all the elements with similar sensitivities. Fangas (Fast Neutron Induced Gamma Spectrometry) has been installed this year, and is now available for the users. We expect it to become useful in the analysis of heavy-metal alloys.

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Presenter: Dr RÉVAY, Zsolt

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

The effect of CsBr doping on the crystallization kinetics of perovskite films

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In recent years, organic-inorganic hybrid perovskite solar cells (PSCs) have made great progress due to the superior optoelectronic properties including high absorption coefficient, high defect tolerance, and long charge carrier diffusion lengths. Benefiting from these excellent properties, the power conversion efficiency (PCE) of PSCs has improved from 3.9% to certified 25.2% with great development prospects. In this work, we demonstrate that doping a small amount of CsBr into the perovskite component, can tune the crystallization behavior and bandgap, promote energy level alignment between perovskite active layer and electron transport layer, and accelerate carrier transport and extraction. In addition, grazing incidence wide angle X-ray scattering (GIWAXS) is used to study the crystal structure and crystal orientation. As a result, we can obtain high performance devices with PCE of 19.24%.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Feasible tuning of microstacking structure and oxidation level in PEDOT: PSS thin films via sequential post-treatment

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Organic semiconductors have attracted intensed attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, PEDOT:PSS is the most studied conducting polymer system in thermoelectric devices due to its intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT and defined as ZT = S2σT/k where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, k is the thermal conductivity, and S2σ is defined as the power factor (PF). However, it is generally considered that it is difficult to obtain a high ZT value of TE materials, due to the fact that the parameters S, σ, and k are interdependent as a function of carrier concentration and hard to be optimized simultaneously. To date, post-treatment is regarded as one promising approach to significantly enhance ZT values of PEDOT:PSS. Herein, PEDOT:PSS thin films are overcoated with salts/DMSO mixtures in order to optimize their TE performance. Subsequently, the surface morphology and the inner morphology are probed, using atomic force microscopy (AFM) and grazing-incidence wide/small-angle X-ray scattering (GISAXS/GIWAXS), respectively. Additionally, UV-Vis spectroscopy, Raman spectroscopy are used to investigate the mechanism behind for TE performance enhancement.

Primary authors: TU, Suo (Institute of Functional Materials); TIAN, Ting; MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: TU, Suo (Institute of Functional Materials)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Effect of Si content within Silicon-Graphite anodes on performance and Li concentration profiles using NDP and conventional electrochemical techniques

Tuesday, December 8, 2020 3:00 PM (25 minutes)

Although addition of silicon to a conventional pure graphite anode leads to a large increase in energy densities, profound morphological changes associated with it, due to repeated (de-)lithiation, may lead to rapid degradation in cell performance. A reversible (de-)lithiation of Li-ions and the formation of a homogenous SEI layer in the initial cycles is therefore crucial.
In this work, we use conventional electrochemical techniques to quantify in-situ the amount of active Li-ions. The electrochemical analysis was conducted using coin-half-cells out of different silicon-graphite (SiG) combinations against lithium chip, as the counter electrode.
Furthermore, we utilized neutron depth profiling (NDP) for an ex situ technique to quantify lithium content, accumulated in SEI as inactive lithium, in different electrode combinations. Here, the coin-half-cells were brought to the desired depth-of-discharges (DODs), using constant current rate of 0.05 h-1. Moreover, the electrodes were extracted and dried under argon atmosphere before conducting the NDP measurements.
The focus lies on the delithiation phase after fully lithiating the electrode samples. Finally, a comparison of Li contents extracted from the two methods is represented. The results show the Li density profiles across the electrode coatings (surface and bulk) for each SiG combination.

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Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

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

Printed block copolymer templated ZnO photoanodes for photovoltaic applications

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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

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Presenter: TIAN, Ting

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Single crystal investigations on the new multiferroic material $LiFe(WO_4)_2$

Thursday, December 10, 2020 1:45 PM (15 minutes)

Multiferroic materials attract much interest during the last decades as the coupling of electric and magnetic ordering offers an application potential for future memory devices or new type of sensors. The most prominent mechanism for multiferroicity is given by the inverse Dzyaloshinskii-Moriya interaction, where a spiral magnetic structure induces a shift of non-magnetic ligand ions and hence a ferroelectric polarization, which can be controlled by the conjugate field of both ferroic ordering parameters. Recently, experiments on a powdered sample of $LiFe(WO_4)_2$ revealed two subsequent magnetic phases, of which the lower one exhibits multiferroic behavior [1]. Beneath $MnWO_4$, $LiFe(WO_4)_2$ is thus the second multiferroic system in this family. Here we report on our single crystal studies on $LiFe(WO_4)_2$ and on the respective structural and magnetic refinements. Neutron diffraction experiments revealed the magnetic structure of both magnetic phases, where first a spin-density wave and subsequently a chiral magnetic structure evolves. Moreover, polarization analysis on the cold three-axes spectrometer KOMPASS unambiguously proves the chiral magnetic phase and shows that even without an external applied electric field a preferred handedness occurrs.
[1] Liu et al. Phys. Rev. B 95, 195134 (2017)

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Session Classification: DN2020: Magnetism

Track Classification: DN: Magnetism

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

Technical design of a levitated dipole for confinement of a low-temperature, long-lived, electron-positron plasma

Wednesday, December 9, 2020 5:40 PM (20 minutes)

A low-temperature, long-lived (LTLL) electron-positron pair plasma has never been produced in a laboratory environment. The APEX project aims to do so by accumulating positrons from the NEPOMUC beam at MLZ and inject them into a magnetic trap formed with a levitated coil in order to study the unique plasma behavior pair plasmas are expected to exhibit. We present technical design plans for this experiment. A closed coil wound with high-temperature REBCO superconducting tape will produce the dipole field. The closed dipole coil (floating coil) will be magnetically levitated by use of a water-cooled copper coil (lifting coil) located above the floating coil. A feedback circuit will vary the lifting coil current in response to input from three laser rangefinders. A cooled radiation shield (RS) insulates the floating coil from room temperature radiation. We estimate a total levitation time on the order of hours. The RS is segmented into eleven electrodes. ExB drift is utilized to move incoming positrons onto closed field lines. The floating coil is mechanically lifted into place and cooled by retracting into a small sub-chamber, which is then pressurized with helium to provide thermal contact with the cold faces. The superconducting charging coil is integrated into this sub-chamber, allowing the floating coil to sit on-plane with the charging coil thus enabling efficient inductive charging. Assembly and first tests with positrons are expected early 2021.

Primary authors: CARD, Alexander (Max-Planck-Institut für Plasmaphysik); STONEKING, Matthew (Max-Planck-Institut für Plasmaphysik); PEDERSEN, Thomas Sunn (Max-Planck-Institut für Plasmaphysik); APEX COLLABORATION (Max-Planck-Institut für Plasmaphysik)

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

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **115** Type: **Poster**

Influence of the scanning strategy on the residual stress state in IN 718 additive manufactured parts

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Laser Powder Bed Fusion (L-PBF) is an additive manufacturing technique enabling the design of complex geometries that are unrivalled by conventional production technologies. Nevertheless, L-PBF process is known to induce a high amount of residual stresses (RS) due to the high temperature gradients present during powder melting by laser. High tensile residual stresses are to be found the edges whereas the bulk material shows balancing compressive RS. Literature shows that the RS is highly sensitive to the process parameters. In particular, this study presents the characterization of the RS state in two L-PBF parts produced with a rastering scan vector that undergoes 90° or 67° rotation between subsequent layers.

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Presenter: Dr SERRANO-MUNOZ, Itziar (BAM)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **116** Type: **Poster**

Precursor engineering of two-step slot-die coated perovskite layers by TBP, MAI and DMSO addition

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The progress of hybrid perovskite materials has amazed the scientific community in the photovoltaic field, demonstrating a rapid progress in the performance within the last 10 years reaching above 25% power conversion efficiency. Now the investigation of ways to move from lab methods (e.g spin-coating) to large-scaled production is required. Those methods include, e.g. roll-to-roll deposition, spray coating or sputtering. One of such roll-to-roll compatible methods is slot-die coating, which has several advantages: low waste of the used material, higher speed of production and possibility to print on a flexible substrate.
To reach highly homogeneous and defect-free, uniform films, two-step methylammonium lead iodide (MAPI) deposition is implemented. 4-tert-butylpyridine-assisted and methylammonium iodide-seeded solutions of lead iodide in dymethylformamide/dimethyl sulfoxide with different ratios as well as their combination are synthesized by slot-die coating with a home-built printer. Surface morphology is altered by addition of this solvents and those changes are investigated by SEM and XRD. Preferential orientation is studied by GIWAXS. Conversion to MAPI is tested and analyzed by XRD.
Results of this work can improve the quality of depositing PbI2-films in two-step perovskite deposition method leading to full conversion of perovskite and better quality of final layer.

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Presenter: SHINDELOV, Oleg

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Conductivity stability of EMIM-DCA post-treated semi-conducting PEDOT:PSS polymer thin films under elevated temperatures

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Nowadays thermoelectric generators are considered a promising technique for heat waste recovery as they enable a direct conversion of a temperature gradient into electrical power. Nevertheless, so far these devices are made of inorganic semiconducting bulk alloy materials like Bi2Te3, which typically contain rare and toxic elements, and are very difficult and expensive to process. Therefore, an increasing research interest is lying on the development of organic TE materials, as these are normally low or non-toxic, lightweight, flexible and enable a large scale, low-cost solution based processability. However, the more recent organic thermoelectric devices cannot compete with the over years well improved inorganic systems. Hence, in this work we are investigating different treatment methods to improve the thermoelectric properties of conducting polymers and try to find a morphology-function relation by measuring parameters such as Seebeck coefficient, electrical conductivity, absorbance, layer thickness and determination of the structure. Hereby, we are also focusing on the effect of different ambient conditions, like temperature or humidity, on the thermoelectric performance.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Separation of the Formation Mechanisms of Residual Stresses in LPBF 316L

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Rapid cooling rates and steep temperature gradients are characteristic of additively manufactured parts and important factors for the residual stress (RS) formation.
This study examined the influence of heat accumulation on the distribution of RS in two prisms produced by Laser Powder Bed Fusion (LPBF) of austenitic stainless steel 316L.
The layers of the prisms were exposed using two different border fill scan strategies: one scanned from the centre to the perimeter and the other vice versa. The goal was to reveal the effect of different heat inputs on samples featuring the same solidification shrinkage. RS were characterised in one plane perpendicular to the building direction at the mid height using Neutron and Lab X-ray diffraction. Thermography data obtained during the build process were analysed to correlate cooling rates and apparent surface temperatures with the residual stress results. Optical microscopy and micro computed tomography were used to correlate defect populations with the residual stress distribution.
The two scanning strategies led to RS distributions typical for additively manufactured components: compressive stresses in the bulk and tensile stresses at the surface. However, due to the different heat accumulation, maximum RS levels differed.
We concluded that solidification shrinkage plays the major role in determining the shape of the RS distribution and the temperature gradient mechanism appears to determine the magnitude of peak RS.

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Presenter: ULBRICHT, Alexander

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Out-of-equilibrium processes during phase transitions: An in-situ crystallization study of hybrid perovskites

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Processes leading up to nucleation are pedantically known to proceed via the emergence of a low-amplitude, long wavelength instability through the material, creating the disturbances for a nucleation process to transpire. Owing to the thermodynamic instability of the high surface energy nanostructures, the nuclei concatenate to form higher surface area intermediates. The processes spanning from the disturbances to the formation of concatenated species occur in the matter of seconds which require high time resolution and sensitivity to register. Thereafter, the conversion of the stabilized concatenated species to the final crystalline material proceed via dissolution-recrystallization which requires further processing steps such as thermal annealing.
By combining in-situ optoelectronic and structural measurements in a custom-made analytical cell, we unveil previously experimentally inaccessible data during non-trivial phase transition processes during the in-situ crystallization of a prototypical hybrid perovskite thin film.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Materials

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

Curvature effects on the stability of lipid bicontinuous cubic phase films interacting with gold nanoparticles

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Non-lamellar lipid membranes are highly relevant in lots of biological processes like exo/endocytosis, and cell division; an interesting case is represented by inverse bicontinuous cubic phase membranes. By designing biologically inspired synthetic bicontinuous cubic phase membranes, it is possible to exploit the amphiphilic nature of their lipid components to encapsulate hydrophobic, hydrophilic and bioactive nanoparticles (NPs) (Nanoscale,2018,10,3480-3488; JCIS 541(2019):329-338). This feature makes them promising candidates as matrices for biosensing applications and the development of NPs-based therapeutic systems. Differently from the case of flat lamellar membranes (J.Microscopy,Ridolfi A.,2020), the interaction of NPs with highly curved cubic membranes has not been extensively addressed yet. We herein present a Neutron Reflectivity (NR) and Grazing Incidence Small Angle Neutron Scattering (GISANS) study on the different structural effects produced by AuNPs of different shapes, when interacting with both cubic and lamellar lipid films. We investigate how variations in the curvatures of both the lipid matrix (lamellar versus cubic phase) and AuNPs (spherical versus rods) influence the stability of the film architecture and the NPs interaction kinetics. In particular, we found that cubic phase films display an increased stability against AuNPs injection compared to lamellar phase films while rod-like AuNPs possess a more disruptive effect compared to the spherical ones.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

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

Micromechanical response of multi-phase Al-alloy matrix composites under uniaxial compression

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Aluminum alloys are extensively used in the automotive industry. Particularly, squeeze casting production of Al-Si alloys is employed in the conception of metal matrix composites (MMC) for combustion engines. Such materials are of a high interest since they allow combining improved mechanical properties and reduced weight and hence improve efficiency. Being a multiphase material, most MMCs show complex micromechanical behavior under different load conditions. In this work we investigated the micromechanical behavior of two MMCs, both consisting of a near-eutectic cast AlSi12CuMgNi alloy, one reinforced with 15%vol. Al2O3 short fibers and the other with 7%vol. Al2O3 short fibers + 15%vol. SiC particles. Both MMCs have complex 3D microstructure consisting of four and five phases: Al-alloy matrix, eutectic Si, intermetallics, Al2O3 fibers and SiC particles.
The in-situ neutron diffraction compression experiments were carried out on the Stress-Spec beamline and disclosed the evolution of internal phase-specific stresses in both composites. In combination with the damage mechanism revealed by synchrotron X-ray computed tomography (SXCT) on plastically pre-strained samples, this allowed understanding the role of every composite's phase in the stress partitioning mechanism. Finally, based on the Maxwell scheme, a micromechanical model was utilized. The model perfectly rationalizes the experimental data and is able to predict the evolution of principal stresses in each phase.

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Presenter: EVSEVLEEV, Sergei

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

Development of an indirect spectrometer Mushroom

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Mushroom is a concept of an indirect neutron spectrometer with its 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, while the value is ca. 0.001 steradian at a TAS. This allows an overview of the dispersion relation and/or diffuse scattering with only a few scans. We report on the theoretical calculations matching the resolution function of the secondary to the primary spectrometer using monochromatised neutrons from one of the neutron guides of FRM II. In addition, the first McStas simulations are presented showing predictions on the instrument performance.

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Presenter: Mr TANG, Ran (Technical Univertsity Munich)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Quantum Phenomena

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

Morphology investigation of printed active layers of hybrid solar cells with grazing incidence neutron and x-ray scattering techniques

Wednesday, December 9, 2020 5:40 PM (20 minutes)

One aspect for the development of non-conventional solar cells should be the sustainability of the production process of devices. Following this idea, we developed hybrid solar cells, which can be processed out of aqueous solution. The active layer of these devices is based on laser-processed titania nanoparticles dispersed in a water-soluble polythiophene. The active layers were produced with a home-built slot die coater. With this printing technique, the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. We investigated the morphology of the deposited active layers with time of flight - grazing incidence small angle neutron scattering (TOF-GISANS) and x-ray scattering. With GISAXS and GIWAXS we were able to follow the evolution of the morphology for different donor/acceptor ratios in situ during the printing process. The expected impact of the observed morphologies and crystallinity on the performance of corresponding devices is discussed.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **124** Type: **Poster**

Hybrid high performance computing to covert the molecular Dynamics simulation to neutron and x-ray data

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The world of computing always strives for a faster solution. The current work made an effort to make the program sassena faster, which calculates the neutron and x-ray.scattering data from atomic simulations, such as molecular dynamics (MD). This can be achieved using different parallelization strategies, e.g. vectorization, thread-based parallelism and distributed memory parallelism. Current work, aided by different analysis tools available on the market, tried to find such opportunities of parallelization within sassena and ensured correctness of the code while implementation of any kind of parallelization. The main goal of this work was to build upon advantages of different parallelism strategies and compensate disadvantages of one strategy by the advantages of others. This work expects a gain in the performance by the use of such a hybrid high-performance computing approach. Furthermore, this work plans to benefit from the achieved performance gain and apply this solution to validate simulations of Hydrogen storage materials with scattering data.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Digitalization and Machine Learning

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

Kinetics of Mesoglobule Disintegration in Aqueous Poly(N-isopropylacrylamide) Solutions Following Pressure Jumps

Thursday, December 10, 2020 4:00 PM (15 minutes)

Stimuli-responsive polymers in aqueous solution form mesoglobules in the two-phase region of the temperature-pressure phase diagram. While the formation of mesoglobules has been amply studied [1], their dissolution and associated structural changes are hardly explored. To elucidate the kinetics of chain swelling and mesoglobule disintegration in a semi-dilute aqueous solution of the thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM), we use in situ, real-time (50 ms –1500 s) small-angle neutron scattering (SANS) at instrument D11, ILL. The coexistence line is crossed by applying a fast pressure jump from the two-phase to the one-phase state, and the target pressure is varied. Two limiting mechanisms are identified: 1) The release of single polymers from the surface of the mesoglobules, leading to a semi-dilute solution. 2) Continuous swelling of the mesoglobules due to uptake of water until the entire system is spanned, resulting in a semi-dilute solution.The first mechanism is dominant when the pressure jumps are carried out in the low pressure regime and when the jumps are shallow. The second mechanism is encountered for deep jumps in the low pressure regime and for all target pressures in the high-pressure regime.

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Presenter: SCHULTE, Alfons (University of Central Florida, Department of Physics and College of Optics and Photonics)

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

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

Failure of the Zimm model: Thermal unfolding of Ribonuclease A

Thursday, December 10, 2020 4:00 PM (15 minutes)

Disordered regions as found in intrinsically disordered proteins (IDP) or during protein folding define response time to stimuli and protein folding times. Neutron Spinecho Spectroscopy is a powerful tool to access directly collective motions of the unfolded chain to observe conformational relaxations. During thermal unfolding of native Ribonuclease A we examine structure and dynamics of the disordered state within a two-state transition model using polymer models including internal friction. The presence of 4 disulfide bonds alters the disordered configuration to a more compact configuration compared to a Gaussian chain that is defined by the additional links. The dynamics of the disordered chain is described by ZIMM dynamics with internal friction between neighboring amino acids. The mode structure is not changed by the additional links, but relaxation times are dominated by mode independent internal friction. Internal friction relaxation times show an Arrhenius like behavior. The dominating internal friction suppresses the characteristics of the ZIMM dynamics and suggest that the characteristic motions correspond to elastic overdamped modes similar to motions observed for folded proteins.

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Presenter: BIEHL, Ralf (Forschungszentrum Jülich)

Session Classification: DN2020: Life Science/ Biology

Track Classification: DN: Life Science/ Biology

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

DNS - diffuse neutron scattering spectrometer at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

DNS is a polarised high intensity cold-neutron time-of-flight spectrometer at MLZ. It is situated between MIRA and SPHERES on neutron guide 6 and uses a wavelength between 2.4 Å and 6 Å. DNS has the capability to allow unambiguous separations of nuclear coherent, spin incoherent and magnetic scattering contributions simultaneously by polarization analysis over a large range of scattering vectors.
It is mainly used for the studies of complex magnetic correlations in frustrated quantum magnets, strongly correlated electron systems, and nanoscale magnetic systems. DNS has a number of unique features such as wide-angle polarization analysis which can be used in parallel to the non-polarization-analyzing position-sensitive detector array covering 1.9 sr.
A 300 Hz disc chopper system for inelastic experiments was commissioned in 2018 and allows an efficient measurements in all four dimensions of S(Q,E). A newly installed Fe/Si based polariser, increased the polarized flux at the sample
position about 50%, largely due to an optimal focussing.

Primary authors: Dr SU, Yixi (JCNS-MLZ); MUELLER, Thomas (JCNS)

Presenter: MUELLER, Thomas (JCNS)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Quantum Phenomena

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

The Absolute Direction of the Dzyaloshinskii-Moriya Interaction in Hematite Determined by Polarized Neutron Diffraction

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Polarized neutron diffraction (PND) is a powerful method which provides direct access to the scattering contribution from nuclear-magnetic interference and thus reveals the phase difference between the nuclear and magnetic structure. This technique can be utilized to gain a detailed insight in the microscopic spin ordering at the unit cell level even for complex magnetic structures. Since magnetic domains correspond to an overall phase shift between the nuclear and magnetic structure, PND also allows to resolve different magnetic domain configurations providing additional information at the mesoscopic scale. This qualifies PND as a versatile tool to simultaneously address a wide range of scientific issues. By conducting a detailed PND study of the prototypical room-temperature weak ferromagnet α-Fe_2O_3 (hematite) we could solve the long standing problem of inconsistent asymmetry signs observed within Friedel pairs in hematite. Moreover, using a detailed symmetry analysis the absolute direction of the Dzyaloshinskii-Moriya interaction (DMI) vector in α-Fe_2O_3 could be determined for the first time. This study is supported by a detailed refinement of the slightly canted magnetic structure and by numerical calculations. It can be used as a reference for further DMI sign determinations, reducing the experimental efforts to the measurement of one representative reflection, making it well suited for highly topical materials often requiring extreme sample environment.

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Presenter: Mr THOMA, Henrik (Jülich Centre for Neutron Science JCNS at MLZ)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

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

New polarized neutron diffraction setup with 8 T magnet on POLI

Thursday, December 10, 2020 2:30 PM (15 minutes)

The polarized single-crystal diffractometer POLI offers two types of polarized neutron diffraction experiments: spherical neutron polarimetry (SNP), also known as full three-dimensional polarization analysis in zero magnetic field, and classical polarized neutron diffraction, also called flipping-ratio (FR) method, in high applied magnetic fields. Recently, the available sample environment of POLI has been extended by an asymmetric field magnet of 8 T. Although this new magnet is actively shielded, its stray fields are still too large to be used with the sensitive ^{3}He polarizer of the original SNP setup. To overcome this issue, a new, large-beam-cross-section solid-state supermirror (SM) bender polarizer has been developed for POLI. An existing shielded Mezei-type flipper is used between the magnet and SM polarizer. A dedicated guide field construction was numerically simulated, optimized and built to link the magnetic field of the polarizer to the flipper and to the stray field of the magnet. An almost loss-free spin transport within the instrument in the complete field range of the new magnet was achieved. The new setup was successfully implemented and tested. A high polarization efficiency of above 99% for short wavelength neutrons could be experimentally reached with the new solid-state bender. The new high–field FR setup is now available for POLI's user community.

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Presenter: Mr THOMA, Henrik (Jülich Centre for Neutron Science JCNS at MLZ)

Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

Contribution ID: **130** Type: **Talk**

Dipolar interactions and spin dynamics in the itinerant ferromagnets Fe and Ni

Tuesday, December 8, 2020 3:25 PM (25 minutes)

Inelastic neutron scattering studies of the spin dynamics of archetypical ferromagnets have been conducted since the invention of those methods. However, the results were limited to relatively large momentum transfers q by experimental difficulties, mainly the coarse resolution of modern TAS or TOF instruments. Utilizing the modern method, a neutron resonance spin echo technique, we investigated the spin-wave dispersion in iron and the paramagnetic spin fluctuations in nickel at small momentum and energy transfer with very high resolution.

The spin wave dispersion of an isotropic ferromagnet is comprehensively described by the Holstein-Primakoff theory, which takes dipolar interactions into account. As expected, the dispersion follows a quadratic form for large q values $E_{SW} \propto q^2$, whereas for small q the dispersion shows linear behavior. This is attributed to the long-range dipolar interaction between the magnetic moments. The subtle influence of these interactions on the magnon spectrum can be expressed by the material specific dipolar wave vector q_D. Hence, the dipolar interactions are primarily probed for $q \leq q_D$.

Our results show excellent agreement with previously conducted triple-axis measurements by Collins et al. in the overlapping regime of q, validating the experimental approach, while extending the investigated range of the spin wave dispersion down to a momentum transfer of $q = 0.015$ $unicodex212B^{-1}$ with unprecedented energy resolution.

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

Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

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

Hybridized crystal field–phonon bound state in cerium-113 compounds

Tuesday, December 8, 2020 4:15 PM (25 minutes)

The coupling between elementary excitations in condensed matter can give rise to novel functional properties and exotic states, such as superconductivity, multiferroicity, or various types of polar order. We are particularly interested in the CeTAl3 (T is a transition metal), family of compounds, for which an unusual bound state was reported in CeCuAl3 and CeAuAl3. It arises due to the magnetoelastic coupling between the crystal field excitation (CEF) and phonons. Although it was observed in few other compounds, e.g. Tb2Ti2O7 [3] or PrNi2 [4], it was reported as an interaction of CEF and an optical phonon, while for CeAuAl3 we have observed an interaction of CEF and strongly dispersive acoustic phonon. This points to a different character of this phenomenon, and awaits a microscopic explanation. We are investigating this effect in other compounds, CePtAl3 and CePdAl3, and its connection with crystal structure and physical properties. In addition we want to determine the influence of the magnetoelastic coupling in Ce-113 compounds on their magnetic ordering and dynamics.
We have conducted various neutron diffraction and spectroscopy measurements on Ce-113 compounds. Our measurements show, that CePtAl3 exhibits a modulated antiferromagnetic ordering below TN=3.35 K, with a modulation vector q=(2/3 0 0), while CePdAl3 orders antiferromagnetically at TN=5.61 K. Magnetic properties, models of magnetic structure and first results on spin and lattice dynamics will be discussed.

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Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

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

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The upcoming high-intensity powder diffractometer ERWIN at MLZ and the cold-neutron powder diffractometer DMC at the Paul Scherrer Institut, Switzerland, will be equipped with new fast and high-resolution two-dimensional position-sensitive curved 3He-based Multi-Wire Proportional Chambers (MWPC) covering 130° horizontal and 14° vertical acceptance. The fully modular design is adopted from a development at Brookhaven National Laboratory (BNL) and consists of nine individual MWPC segments mounted seamlessly inside a common pressure vessel filled with a gas mixture of 6.5 bar 3Helium + 1.5 bar CF4. The device with a radius of curvature R = 800 mm is aiming at 75% detection efficiency for thermal neutrons, 1.6 mm x 1.6 mm position resolution (FWHM) and about 200 kHz count rate capability per MWPC segment at 10% event loss. Single channel induced charge readout using a Time-over-Threshold detection method is applied to the 1152 x 1152 individual cathode wires and strips, respectively. For each detected neutron a FPGA-based signal processing electronics developed in-house will provide 2D-position information applying a Centre-of-Gravity algorithm and time stamping with 80 ns time resolution.
First results of measurements performed with a 30°-prototype using a collimated beam of 4.73 Angstrom neutrons at the TREFF instrument at FRM II and the present status of the construction of the full size detectors will be presented.

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Presenter: Dr ZEITELHACK, Karl (MLZ)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

Altering of PNIPAM microgels: pressure vs. temperature

Tuesday, December 8, 2020 5:35 PM (25 minutes)

Poly(*N*-isopropylacrylamide)(PNIPAM) is a classical representative of stimuli-responsive polymers in various polymer systems like microgels, brushes, micelles [1-2]. Application of external stimuli such as temperature or pressure induces structural alterations of the polymer systems. It makes them the promising candidates for various application. However, the polymer parameters and the polymer phase transition strongly depends on the applied trigger and a detailed understanding of the stimuli-induced processes is of high demand.
Since PNIPAM is known to be thermo-responsive, T-induced transition of homopolymer gels as well as PNIPAM-based microgels is widely studied. In turn, the knowledge of pressure driven transition of PNIPAM microgels is still limited. We thus present the structural investigation of the cross-linked PNIPAM microgels within a wide pressure-range (0–5 kbar) at different temperatures by means of VSANS using a sapphire windows HP-cell for liquids at the KWS-3 instrument (JCNS at MLZ). The temperature- and pressure-increase leads to the change of the structural parameters of the PNIPAM microgels, for instance a difference in p- and T-driven transition was found. The results of the effect of the temperature and pressure on the above mentioned system will be presented and the temperature dependence of the pressure point at the phase transition will be discussed.
[1]T. Kyrey et al., Soft Matter (2019) 15, 6536
[2]J. Witte et al., Soft Matter (2019) 15, 1053

Primary authors: Dr KYREY, Tetyana (JCNS at MLZ, Forschungszentrum Jülich GmbH); PIPICH, Vitaliy; APPAVOU, Marie-Sousai (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH); WITTE, Judith (TU Berlin); FÖRSTER, Stephan (Forschungszentrum Jülich)

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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

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

A tensile rig for neutron imaging

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Electrical steel sheets are used as the magnetic cores of electric engines. Stress in such sheets causes energy loss during the reversal of magnetization due to the magneto-elastic effect, which can be used to guide the magnetic flux. Such change in the magnetic properties can be detected by neutron grating interferometry (nGI), which allows to map ferromagnetic domains in bulk materials [1].
Previously, the effects of residual stress in electrical steel sheets, introduced through embossing, were investigated [2,3].
Now a more realistic case for electric engines is planned to be tested by replicating the effects of alternating magnetic fields and centrifugal forces.
Hence, a custom tensile rig for the nGI setup of the ANTARES beamline was built.
The new tensile rig in combination with a newly constructed magnetic yoke allows to place sheet metal samples in the nGI setup at varying levels of mechanical strain while simultaneously applying static or alternating magnetic fields. Therefore, the effects of overlapping centrifugal tensile strain and residual stress from embossing of electrical steel sheets can be evaluated.
The tensile rig can furthermore be used with different inserts to accommodate arbitrarily shaped samples.

[1] C. Grünzweig et al., APL 93, 112504 (2008)
[2] S. Vogt et al., Production Engineering 13.2 (2019), pp. 211-217
[3] H. A. Weiss et al., Journal of Magnetism and Magnetic Materials 474 (2019), pp. 643-653

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

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

Targeted use of residual stresses in electric sheet to increase energy efficiency

Thursday, December 10, 2020 4:15 PM (15 minutes)

Electrical steel sheets are used in electric drives to guide the magnetic field and their efficiency strongly depends on energy losses during the reversal of magnetization. The energy loss is coupled to the mobility of the magnetic domains, which is negatively affected by stress caused during the manufacturing process [1, 2].
Neutron grating interferometry (nGI) allows to probe the bulk local magnetic properties in samples of technically relevant dimensions, which is not possible with most other techniques by tracking the amount of ultra-small-angle-neutron scattering inside a sample [3]. The DFI image is related to the distribution and size of magnetic domains inside a sample serving as possible scattering centers and allows to track the degradation of magnetic domain wall mobility caused by stress.
In this project we use the degradation of the magnetic domains by targeted stress to actively guide the magnetic field, allowing to build more efficient electrical drives. We will give a overview about the achieved results in flux guidance using various embossing strategies. Moreover we present an outlook on future experiments.
This project is a collaboration with the utg (TUM) and IEM (RWTH Aachen) as part of the DFG priority program SPP2013
[1] H. Weiss et al., J. Magn. Magn. Mater. 474, 643 –653 (2018)
[2] A. Moses, IEEE Trans. Magn, Vol. 15, 1575-1579 (1979)
[3] C. Grünzweig, PhD thesis (2009)

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Presenter: NEUWIRTH, Tobias

Session Classification: DN2020: Materials

Track Classification: DN: Materials

Contribution ID: **136** Type: **Poster**

URANOS - a voxel engine Neutron Transport Monte Carlo Simulation

Wednesday, December 9, 2020 5:40 PM (20 minutes)

URANOS (Ultra RApid Neutron-Only Simulation) is a newly developed 3D neutron transport Monte Carlo from thermal to fast energy domains. Emerging from a problem solver for the CASCADE detector development in collaboration with environmental physics the project aims towards providing a fast computational workflow and an intuitive graphical user interface (GUI) for small to medium sized projects. It features a ray-casting algorithm based on a voxel engine. The simulation domain is defined layerwise, whereas the geometry is extruded from a pixel matrix of materials, identified by specific numbers. Therefore, input files are solely a stack of pictures, all other settings, including the configuration of predefined sources, can be adjusted by the GUI.
The scattering kernel features the treatment of elastic and inelastic collisions, absorption and absorption-like processes like evaporation. Cross sections and distributions are taken from the data bases ENDF/B-VII.1 and JENDL/HE-2007. In order to simulate multi-layer boron detectors it also models the charged particle transport following the conversion by computing the energy loss in the boron and its consecutive layer.
URANOS is freely available and can be used to simulate the response function of boron-lined or epithermal neutron detectors, small-scale laboratory setups and especially transport studies of cosmic-ray induced environmental neutrons.

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Presenter: Dr KÖHLI, Markus (Heidelberg University)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **137** Type: **Poster**

Phase analysis of steel using neutron grating interferometry and bragg edge imaging

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Austenitic steel transforms to martensite under applied strain. An undesired modification of the mechanical properties by this process is typically compensated by annealing to restore the austenitic phase. Recently, it has been proposed to introduce a beneficial residual stress state in the material.
A spatially resolved determination of the phase fractions of martensite is required for the quantification of local residual stress introduced by manufacturing [1,2].
We non-destructively tracked the amount of martensite inside drawn austenitic steel samples using neutron bragg edge imaging (BEI) and neutron grating interferometry (nGI).
Differentiation between the two phases is possible by BEI due to their different crystal structure but complicated by strain induced texture.
nGI on the other hand is sensitive to scattering off ferromagnetic domains composed of martensite inside the material [3].
To verify the results of the two techniques we compared them to surface micrographs of the samples.

[1] M. Baumann, A. et al., MATEC web of Conferences 190, 2018
[2] K.A. De, et al., Scripta Materialia 50, pp. 1445-1449, 2004
[3] F. Pfeiffer et al., PRL, 96.21 (2006), 215505

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Presenter: NEUWIRTH, Tobias

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Materials

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

Protein Short-Time Diffusion in a Naturally Crowded Environment

Thursday, December 10, 2020 4:15 PM (15 minutes)

Macromolecular crowding, i.e. the presence of macromolecules at high volume fractions, affects reaction rates and transport processes in the cell. For reliable quantitative models of cellular pathways, the mobility of individual proteins is thus a key information. Often, the protein mobility is modeled by the self-diffusion of colloidal systems. The underlying assumption that neither the shape and size of proteins nor the polydisperse nature of the cytosol matters, has not been checked experimentally so far.
Here, we present a combined experimental-simulational study on the mobility of tracer proteins in cellular lysate [1]. Using quasi-elastic neutron backscattering, we study the mobility of immunoglubulin in deuterated cellular lysate from E.coli. Varying the mixing ratio and volume fraction of protein and lysate, we observe that the immunoglubulin mobility depends on the total volume fraction only. Using Stokesian dynamics simulations, we calculate the mobility of tracers in a model system for the lysate. In the polydisperse lysate, proteins with an average size indeed are slowed down similar to a monodisperse solution of same volume fraction, whereas larger/smaller proteins diffuse slower/faster, respectively. As immunoglubulin is close to the average size, we obtain a consistent picture on the protein mobility in a polydisperse cell-like environment, which is promising for a future quantitative understanding of reaction pathways.
[1] Grimaldo et al. JPCL 2019, 10, 1709

Primary authors: GRIMALDO, Marco (Institut Laue-Langevin, Grenoble, France); Dr LOPEZ, Hender (TU Dublin - School of Physics & Clinical & Optometric Sciences); BECK, Christian (Institut Laue Langevin); ROOSEN-RUNGE, Felix (Faculty of Health and Society, Malmö University, Sweden); MOULIN, Martine (Institut Laue Langevin, Grenoble, France); DEVOS, Juliette (Institut Laue-Langevin); LAUX, Valerie (Institut Laue Langevin,Grenoble, France); HÄRTLEIN, Michael (Institut Laue Langevin, Grenoble, France); DA VELA, Stefano (EMBL Hamburg, Germany.); SCHWEINS, Ralf (Institut Laue - Langevin); MARIANI, Alessandro (ESRF, Grenoble, France); ZHANG, Fajun (University of Tuebingen); BARRAT, Jean-Louis (Universite Rhone Alpes, Grenoble, France); OETTEL, Martin (Institut für Angewandte Physik, Universität Tübingen, Germany); FORSYTH, Trevor (ILL); SEYDEL, Tilo (Institut Max von Laue - Paul Langevin); SCHREIBER, Frank (Institut für Angewandte Physik, Universität Tübingen, Germany)

Presenter: ROOSEN-RUNGE, Felix (Faculty of Health and Society, Malmö University, Sweden)

Session Classification: DN2020: Life Science/ Biology

Track Classification: DN: Life Science/ Biology

Contribution ID: **139** Type: **Poster**

Boron-lined tubes and readout electronics for low count-rate environments

Wednesday, December 9, 2020 5:40 PM (20 minutes)

With Boron-10 converters replacing helium-3 the total sensitive detector area per instrument increased likewise due to the lower efficiency per layer. However, commonly used alloys for substrates contain a significant amount of radioisotopes which lead to an undesired background counting rate. For detector applications exposed to a low flux, like in our case measuring environmental neutrons generated by cosmic-ray particles, such can easily increase the error of the signal. The tubes we have developed feature B4C coatings of up to 0.2 m2 on high-purity copper substrates. Furthermore the geometry and the pressure have been designed for a dE/dx suppression of unwanted contributions from gammas, electrons, muons and also heavy-isotope decays like from remains of radon. In combination with the form factor our pulse shaping electronics determines pulse length and height, which allows to discriminate against other particle species. The main goal of this development is to provide a detector system largely free of intrinsic background at considerably lower costs.

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Presenter: KÖHLI, Markus (University of Heidelberg)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Neutron imaging for the investigation of the lyophilisation of amorphous bulk solids

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Lyophilisation refers to the sublimation of ice below the triple point of water. It is employed for dehydrating biopharmaceuticals and high-value foods in frozen state as the structural and nutritional attributes are not affected. The sublimation front divides the dried area from the frozen area. The knowledge about the sublimation front is important to understand process characteristics and to ensure the product quality. However, the development of the sublimation front, especially in particulate matter, is not yet fully understood and the existing models are contradictory and based on different assumptions. No experimental validation of the existing models exists so far. Therefore, it is the aim to study the sublimation front by in-situ neutron imaging.
The experiments were carried out in the Antares beamline at FRMII using maltodextrin particles of two different particle sizes and concentrations. Sublimation for finer particles (x= 70 µm) was investigated by radiography. For the larger particles (x = 3550 µm) continuous tomographic measurements were carried out.
With the reconstructed 3D volumes, we could demonstrate the structure of the drying fronts, whereas with the radiographic images we could estimate the dynamic ingress of the sublimation front. It was shown that for small particles the sublimation front first occurred at the bottom of the particle bed and moved to the top. For large particles multiple sublimation fronts were found.

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Presenter: FOERST, Petra (TUM)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

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

In situ light scattering techniques at neutron instruments at the MLZ - experiences made and challenges ahead

Wednesday, December 9, 2020 5:40 PM (20 minutes)

What is well established at many synchrotron beam lines is still in the development phase at neutron instruments: in situ light scattering techniques for on-beam sample control. Biological samples often show a sufficiently broad spectral range where light absorption does not play a dominant role. This enables in situ sample control using dynamic and static light scattering techniques. Many biological samples undergo a slow aggregation process during the comparatively long neutron data collection times. If the aggregates are staying few in number and/or if their form factor has decayed enough in the relevant q-range, the neutron measurement can be continued. If not, a fresh sample can be used.
Candidates for neutron instruments to be equipped with an in situ light scattering set-up are small angle scattering, spin echo, time-of-flight and backscattering instruments operating sample environments near or at room temperature. We routinely provide in situ dynamic light scattering with one fixed scattering angle at the instrument KWS-2 at MLZ to interested users. For the Jülich spin echo spectrometer J-NSE we have developed a temperature-controlled sample environment which includes two laser colours and three light scattering angles. This not only enables dynamic light scattering but also static light scattering at six different q-values is feasible.
This contribution discusses the experiences made with these in situ set-ups and looks into future developments and improvements.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

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

LLZO: Al, Ta, Nb, W –different dopants and their effect on microstructure and lithium diffusion

Wednesday, December 9, 2020 5:40 PM (20 minutes)

To understand the impact of different dopants (Al, Ta, Nb, W) on the structure and ion conductivity of the solid electrolyte LLZO (Li7La3Zr2O12) on all length scales, we performed XRD, X-PDF, 6Li NMR and neutron diffraction experiments. The dopants Nb and Ta yielded cubic structured LLZO with highest ionic conductivities amongst this class of solid state electrolytes. Additionally, we observed that mechanical treatment of these materials cause a symmetry reduction : $Ia\bar{3}d \rightarrow I4\bar{3}d$ and a geometrically frustrated local structure. To understand the impact on the Li ion conductivity, neutron powder diffraction and 6Li-NMR were utilized. To this end, impedance spectroscopic and temperature dependent 6Li NMR measurements are used to determine the Li ion conductivity. Despite the finding that, in some materials, disorder can be beneficial, with respect to ionic conductivity, pulse-field gradient NMR measurements of the long-range transport up to 500 µm indicate a bulk Li+ diffusion barrier in the lower symmetric structure. The geometric frustration and symmetry reduction can be cured and converted back into the higher symmetric garnet structure by temperature treatment. The Li+ conductivity enhancing effect of the temperature treatment is proven by impedance measurements of sintered pellets.

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Presenter: FRITSCH, Charlotte

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **143** Type: **Talk**

Magnetic structure of the Mn moment in the magnetic weyl Semimetal Mn3Sn

Tuesday, December 8, 2020 3:50 PM (25 minutes)

In the last few years, Mn3Sn has shown a large interest in condensed matter physics community due to the Weyl Semimetallic nature of this compound. Due to the emergent Berry flux from the Weyl points, Mn3Sn shows interesting properties like Anomalous Hall Effect, Chiral magnetic effect, and other non-local transport properties.
Along with exotic transport properties, this material shows temperature-dependent magnetic structure. To understand the connection between Weyl properties with the magnetic structure we have performed single crystal neutron diffraction of Mn3.17Sn sample at the HEiDi instrument at FRM II. Our diffraction experiment confirms that between 274 K < T < 420 K (TN) Mn moment order in an inverse triangular antiferromagnetic structure in the a-b plane. In the temperature range 50 to 274 K, Mn moments order in a spiral magnetic structure. The same spiral magnetic structure persists below 50 K down to 4 K where a spin-glass state was reported. The direct correlation between the magnetic structure and the Anomalous Hall Effect (AHE) is still unclear. As few groups claimed that in the incommensurate region (50 K to 190 K)1 no AHE was observed but other groups found AHE in this region2. We have observed AHE in the incommensurate region with amplitude compare to the published report.

Reference:
1. N. H. Sung et al. Applied Physics Letter 112, 132406 (2018).
2. S. Nakatsuji et al. Nature 527, 212 (2015).

Primary author: JANA, SUBHADIP

Co-authors: Mr RAI, Venus; NANDI, Shibabrata (JCNS2); Mr PERSSON, Jörg (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, Germany); MEVEN, Martin (RWTH Aachen University, Institute of Crystallography - Outstation at MLZ); DUTTA, Rajesh (Institut für Kristallographie, RWTH Aachen University); BRÜCKEL, Thomas (Forschungszentrum Jülich GmbH)

Presenter: JANA, SUBHADIP

Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

Contribution ID: **144** Type: **Talk**

Critical magnetic fluctuations in Ca2RuO4 studied by neutron spin-echo and triple-axis spectroscopy

Thursday, December 10, 2020 2:00 PM (15 minutes)

We report on comprehensive high-resolution linewidth measurements of critical antiferromagnetic fluctuations in Ca_2RuO_4 (CRO214) performed at the neutron resonance spin-echo spectrometer TRISP at FRM II and the cold triple-axis spectrometer FLEXX at BER II. CRO214 is structurally related to the unconventional superconductor Sr_2RuO_4 [1] and hosts a complex interplay between magnetic and electronic correlations leading to a novel type of soft-magnetism with strong single-ion anisotropy, and 'Higgs'amplitude fluctuations in the spin-wave spectrum, as revealed by recent neutron experiments [2].
In contrast to conventional magnetic phase transitions, the magnetic ordering in CRO214 below T_N ~ 110 K emerges from exciton condensation [3]. Therefore, since the magnetic fluctuations in proximity to T_N are fundamentally related to the nature of the magnetic correlations in the system, our study can shed new light on the exceptional 'excitonic'magnetism in CRO214.

[1] Nat. 372, 532, (1994).
[2] Nat. Phys. 13, 633, (2017).
[3] Phys. Rev. Lett. 111, 197201, (2013).

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Session Classification: DN2020: Magnetism

Track Classification: DN: Magnetism

Contribution ID: **145** Type: **Talk**

Spin-liquid-like state in anion-disordered $Gd_2Hf_2O_7$

Tuesday, December 8, 2020 2:05 PM (25 minutes)

Pyrochlore antiferromagnets (AFM) $Gd_2T_2O_7$ (T: tetravalent metal elements) are prototypical materials for realizing classical spin liquid states. However, most of them have been observed to show long-range magnetic order. Previous studies show that $Gd_2Hf_2O_7$ has Curie-Weiss temperature ≈ -7.3 K and a tiny sharp peak on the top of a large broad maximum in the specific heat data indicating a long-range AFM order. Here we present our investigation on the nuclear and magnetic structures of $Gd_2Hf_2O_7$. Using neutron diffraction, we found that the sample has $\sim 8\%$ oxygen Frankel defects with undetectable Gd/Hf antisite defects. The polarized neutron diffuse scattering pattern shows liquid-like scattering at 30 mK without any magnetic Bragg peaks, evidencing a spin-liquid-like ground state. The pattern was further analyzed using reverse Monte Carlo method together with unsupervised machine learning techniques, which reveals a Palmer-Chalker order over the range of a single unit cell. Bond disorder due to oxygen anion disorder may be responsible for the absence of long-range order.

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Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

Contribution ID: **146** Type: **Talk**

Structure-dynamics relation in Zr-Ti melts

Thursday, December 10, 2020 3:30 PM (15 minutes)

The early transition metals Zirconium and Titanium show very similar chemical and structural properties. The binary Zr-Ti alloys compose a completely miscible system, which is also a boundary system for many bulk metallic glasses (BMGs) and stable quasicrystals. However, the detailed formation mechanisms of these special structures remain largely unknown and are often speculative, since for these chemically reactive, high melting temperature alloys accurate knowledge of melt properties is largely missing. Using containerless levitation techniques, we successfully investigated the microscopic structure and dynamics of the Zr-Ti melts over a large temperature range. Neutron and synchrotron diffraction experiments reveal a melt structure exhibiting barely any chemical short-range order. On the Zr-rich side, the Ti diffusivity obtained by quasi-elastic neutron scattering decreases with increasing Ti content. Such a concentration dependent atomic dynamics can be fully understood according to the prediction of the Mode-Coupling Theory (MCT) on a binary hard-sphere mixture with a small size disparity. Our results indicate the dominant impact of the topological structure on the atomic motion in the Zr-Ti melts.

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Session Classification: DN2020: Materials

Track Classification: DN: Materials

Contribution ID: **147** Type: **Poster**

Injection of positrons into an electron space charge in a dipole field

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Towards the goal of magnetically confined low-energy electron-positron plasmas, the APEX collaboration has already demonstrated significant progress in injecting and confining the high-flux reactor-based positron beam, produced in the NEPOMUC facility. As previous work had focused on the single-particle regime, questions on the role of collective effects on positron injection via ExB drift needed to be investigated. Therefore a thermionic source installed on the equatorial plane of the dipole trap continuously injects electrons into the confinement volume and creates a negative space potential. Around 10% of the emitted electrons are confined in the magnetic field and contribute in establishing an additional potential as low as -58V in the injection area of the 5eV positron beam. Certain potential configurations increase the parameter range that allows successful positron injection while preserving the 100% efficiency. An overview of
the APEX project, the effect of this additional potential on the injection process of positrons as well as the diagnostic system consisting of target probes, gamma detectors and an emissive probe will be presented in this contribution.

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Presenter: SINGER, Markus

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **148** Type: **Talk**

Magnetic structure of the frustrated fcc iridate (NH4)2IrCl6: A candidate J_eff=1/2 Mott insulator

Thursday, December 10, 2020 2:15 PM (15 minutes)

Magnetic materials containing octahedrally coordinated Ir^{4+} ions can give rise **novel J_{eff} =$\frac{1}{2}$ magnetic moments** due to the interplay of **strong spin-orbit coupling**, onsite Coulomb repulsion and crystalline electric field. The exchange interaction between such moments depends on the geometry of the exchange paths between the magnetic ions and could be **highly anisotropic** such as the **Kitaev exchange** in 2D honeycomb lattice. This could lead to a rich variety of magnetic ground states with **exotic excitation** as has been proposed theoretically and also observed experimentally in several real materials. $(NH_4)_2IrCl_6$ retains its cubic symmetry (fcc) down to very low temperatures and offer best possible condition for the cubic crystalline electric field to realize genuine J_{eff} =$\frac{1}{2}$ state. The crystal and magnetic structures of the $(NH_4)_2IrCl_6$ single crystal have been studied using neutron diffraction, synchrotron X-ray diffraction and resonant inelastic X-ray scattering techniques. The study shows that the interplay of geometrical frustration and the bond dependent exchange frustration stabilizes a type-III collinear AFM ordering at T_N=2.1 K with propagation vector (1 $\frac{1}{2}$ 0). Thus **the bond dependent Kitaev interaction in the fcc lattice may oppose the magnetic frustration** which is in sharp contrast to the Kiteav interaction in honeycomb lattices promoting quantum spin-liquid ground states.

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Session Classification: DN2020: Magnetism

Track Classification: DN: Magnetism

Contribution ID: **149** Type: **Poster**

Comparison of guide systems for instruments at the high brilliance source (HBS)

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Compact accelerator-based neutron sources (CANS) have the potential to generate neutron beams for scattering studies comparable to research reactors. Such a source is currently developed at Jülich Centre for Neutron Science (JCNS). It is expected to provide thermal and cold neutrons with high brilliance and is therefore called "High Brilliance Source"(HBS). In this framework, the performance of neutron guide systems for the instrument are studied. The guide for a medium resolution time-of-flight diffractometer for nano-scaled and disordered materials, suggested for the HBS, was identified as a typical example. Different shapes of this guide have been simulated, namely an elliptical shape and ballistic shapes with elliptical diverging/converging sections of two different lengths. The moderator-guide distance has been varied between 30 and 140 cm for two different entry cross-sections using the CANS feature to bring the optics very close to the slow neutron source.
The results show that neutron beam properties at the sample position have a strong dependence on the geometry of the guide system, especially the distance from moderator to guide entry. Also, under these conditions - small source and short moderator guide distance - a ballistic guide with a long elliptical converging/diverging part has a performance comparable to that of an elliptical guide and is thus the most promising candidate for such a diffractometer.

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Presenter: MA, Zhanwen (Jülich Centre for Neutron Science JCNS Forschungszentrum Jülich GmbH)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

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

Micromechanics near the yield point of Nickel based superalloys

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Previous studies found non-monotonous lattice strain evolutions at small plastic deformations in the Nickel-based superalloys Inconel 718 and Haynes 282. For studying the micromechanical causes of this behaviour, the dependence of these effects on dislocation density, deformation history, and temperature history was examined. Due to the material‘s more readily observable non-monotonous lattice strain evolutions (when compared to Inconel 718), the material Haynes 282 was given special attention. In situ bulk diffraction experiments in the regime of small plastic strains yielded repeatable, non-monotonous strain evolutions, repeatable peak sharpening during unloading and no strong dependence on conditions typically expected to promote solute atom segregations to dislocation. The observed micromechanical softening is accompanied by strain localization (observable by slip band formation) and dynamic strain ageing at elevated temperatures.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **151** Type: **Poster**

In situ neutron dilatometry investigation of βo→β phase transformation in TiAl alloys

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Intermetallic TiAl alloys represent a novel class of lightweight high temperature materials for applications in aero and automobile industries. One of their most impressive example of use is replacing the twice as dense Ni-based turbine blades in the last stages of the aero engine in the Airbus A320neo family, yielding to a decrease of noise and CO2 emission.
Nevertheless, there is need for improvements e.g. in processing for higher cost effectivity and better material behavior at the working temperatures. Advanced TiAl alloys are particularly well suited for hot working due to the presence of the ductile, disordered, body-centered cubic (bcc) β phase (A2 structure) at high temperatures. However the challenge to be met is to avoid presence of the so-called "ordered beta"βo phase (B2 structure), which is brittle at service temperature and decreases the turbine blades lifetime.
Our current project is a fundamental investigation of βo→β phase transformation in TiAl and its dependency from different β-stabilizing elements. We used the new dilatometer DIL 805AD as an in situ sample environment at STRESS-SPEC (FRM II, Garching bei München) for stepwise heating experiments in the temperature range from 1000℃ up to 1400℃. The results unambiguously determined the presence of the βo phase and the transformation temperatures of βo→β. The results will be compared with synchrotron measurements performed with the same type of dilatometer under a better time resolution.

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Presenter: KONONIKHINA, Victoria (Helmholtz-Zentrum Geesthacht)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **152** Type: **Talk**

Insights into the (de)lithiation mechanism of core-shell layered Li(Ni,Co,Mn)O2 cathode materials during cycling

Tuesday, December 8, 2020 2:05 PM (25 minutes)

Layered LiNixCoyMn1-x-yO2 (NCM) oxides with core-shell morphology have been found to be prospective cathode candidates for advanced lithium-ion batteries. The electrochemical performances of NCM cathodes are tied to the transition metal relative ratios, thereby it is difficult to determine the real structure of core-shell NCM materials and to understand the synergistic effect of core and shell upon cycling. Herein, high-resolution neutron powder diffraction at the instrument SPODI was used to investigate the structure of synthesized NCM compound. The results show that the as-prepared NCM material consists of an inner Ni-rich core and a Mn-rich shell on a secondary particle level. Both core and shell possess a layered α–NaFeO2–type structure with the same space group ($R\bar{3}m$) while a slight difference in lattice parameter. The (de)lithiation mechanism of core-shell NCM cathode materials was investigated by in situ synchrotron-based X-ray diffraction and absorption spectroscopy. These findings contribute to prepare layered Ni-based oxides with good electrochemical performances.

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Presenter: HUA, Weibo (Karlsruhe Institute of Technology (KIT))

Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **153** Type: **Talk**

In-operando neutron reflectometry reveals the solid electrolyte interface formation on surface coated silicon based anodes for lithium-ion batteries

Tuesday, December 8, 2020 4:15 PM (25 minutes)

Silicon anodes for lithium ion batteries (LIBs) exhibit a high theoretical capacity of 3590 mA h g^{-1} –one magnitude higher than commonly used graphite –but they suffer a large volume expansion of around 300 % during cycling. The formation and composition of the solid electrolyte interface (SEI) in LIBs has a huge impact on the stability and performance of the cell. Coatings of only 10 nm have a large influence on the SEI and therefor on the stability of the silicon based anode, hence also the cell.[1] Static time-of-flight neutron reflectometry (TOF NR) measurements proof the first three cycles sufficient to form the SEI using metallic lithium as counter electrode. Carbon or TiO_2 surface coatings on $Si_{85}Ti_{15}$ alloy anodes significantly influence the composition and thickness of the SEI. In-operando TOF NR measurements during cycling lead to a better fundamental understanding of the formation and growth of the SEI on these high-performance LIB anodes.

References
(1) Xie, H.; Sayed, S. Y.; Kalisvaart, W. P.; Schaper, S. J.; Müller-Buschbaum, P.; Luber, E. J.; Olsen, B. C.; Haese, M.; Buriak, J. M. Adhesion and Surface Layers on Silicon Anodes Suppress Formation of c -Li 3.75 Si and Solid-Electrolyte Interphase. *ACS Appl. Energy Mater.* **2020**, *3*, 1609–1616.

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Presenter: SCHAPER, Simon J.

Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

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

Morphology of fullerene-free bulk heterojunction blends for photovoltaic applications

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Over the last decades, the focus of research has been shifted towards the field of organic electronics due to their advantageous properties, such as low-cost manufacturing processes, versatility, flexibility, as well as their tunable characteristics, such as absorption and solubility. These properties open up a wide range of applications, especially, in the field of photovoltaics. Hence, organic photovoltaics represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 16% have been reported and thus receive industrial attention for commercialization. We study the inner morphology of a low band gap, fullerene-free bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural information is correlated with current density voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

Contribution ID: **155** Type: **Talk**

Neutron PDF for insight into hydration shells around iron oxide nanoparticles

Tuesday, December 8, 2020 2:05 PM (25 minutes)

Interfaces between iron oxide nanoparticles (IONP) and water are of great importance in various fields spanning biomedicine, waste water treatment and catalysis. Recently, we could distinguish adsorbed water species and extended hydration layers around IONPs via a double-difference X-ray pair distribution function (dd-PDF) analysis.1 Details of the interfacial hydrogen bond network shall now be addressed with neutrons.
Here we present neutron total scattering data on IONP powders and their aqueous dispersions (H2O/D2O), to which we apply our dd-PDF strategy.1 7 nm sized IONPs are synthesized in basic diethylene glycole and capped with citrate or phosphocholine. We developed a transferable, robust combination of TGA, AAS and elemental analysis to determine the exact composition of the powders, especially amount of the organic capping agents, important for absolute normalization of the neutron data.2 Additionally, contributions of surface-OH (-OD) groups of wet powders with varying amount of surface water layers are investigated according to 3.
Finally, we aim at elucidating interfacial structures like surface hydroxyls, ligand coordination and possibly contributions from in-plane co-adsorbed water molecules, via a contrast match study to bridge the gap between insight into wet powders and colloidal dispersions.

1. Thomä, S. L. J. et al., Nat. Commun. 2019, 10(1), 995.
2. Eckardt, M. et al.,in preparation
3. Wang, H. et al., J. Am. Chem. Soc. 2013, 135, 6885-6895

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Presenter: THOMÄ, Sabrina (Universität Bayreuth)

Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **156** Type: **Talk**

Compact Clamp Cells for High Pressure Neutron Scattering at Low Temperatures and High Magnetic Fields at MLZ

Tuesday, December 8, 2020 3:50 PM (25 minutes)

The combination of high pressure, low temperature and high magnetic fields with neutron scattering is of great interest for the study of a wide range of materials, e.g. quantum phenomena where competing magnetic interactions are tuned by pressure. The basic requirement for such experiments is the availability of suitable pressure devices. The most common type of device for high-pressure neutron experiments is the *clamp cell*: the pressure is applied and fixed *ex-situ*, allowing an independent use of the same cell/sample in various setups.

Here we report on the development of dedicated compact clamp cells for neutron scattering experiments in the closed-cycle cryostats and high-field magnets on the beamlines DNS, MIRA, and POLI. The cell has been produced in CuBe and in NiCrAl variants, working up to about 1.1 GPA and 1.5 GPa, respectively, in good agreement with theoretical predictions. The use of nonmagnetic materials allows measurements of magnetic properties of the sample in both cells even using polarized neutrons.
First tests in the CuBe cell have been successfully performed for the load/pressure calibration curve, cell attenuation and background measurement both with cold and hot neutrons, and to test thermal behavior, measuring magnetic reflections at very low temperatures. The results of these tests will be presented. The new cells are well suited for high pressure measurements at ultra-low temperatures and in combination with an applied magnetic field.

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Presenter: Mr EICH, Andreas (Forschungszentrum Jülich GmbH; RWTH Aachen)

Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **157** Type: **Poster**

Cononsolvency-Induced Collapse Transitions in Thin PMMA-b-PNIPAM and PMMA-b-PNIPMAM Films

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Stimuli responsive thin films combine the advantages of polymers in bulk, i.e., their increased stability and of polymer solutions, i.e., their fast response and therefore are attractive for a wide range of applications. Towards future applications, we investigate the not yet well understood phenomenon of cononsolvency. For this we prepared thin films of the thermoresponsive diblock copolymers PMMA-*b*-PNIPAM and PMMA-*b*-PNIPMAM which exhibit cononsolvency induced collapse transitions when organic cosolvents, like acetone or methanol, are introduced into the surrounding atmosphere. The chemical structures of NIPAM (*N*-isopropylacrylamide) and NIPMAM (*N*-isopropylmethacrylamide) differ by an additional methyl group, which is able to influence the film collapse kinetics on a macroscopic scale. The macroscopic changes during the swelling and collapse transitions were investigated by spectral reflectance (SR) and verified through time-of-flight neutron reflectometry (ToF-NR) measurements. On a more molecular level we further elucidate the underlying mechanism by *in situ* Fourier-transform infrared spectroscopy (FTIR) measurements to gain further insight into the origin of the cononsolvency effect.

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

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **158** Type: **Poster**

Structure and dynamics of polyelectrolytes in water solution

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Intrinsically disordered proteins (IDP) challenge the classical structure function paradigm in structural biology as they have specific function without fixed structure. Specifically, the dynamics of flexible chains seems to be of great importance for fast response to environmental conditions. Since proteins and, in particular, IDPs have properties of charged polymer chains, polyelectrolytes (PE) can be used as model system to study response of charged chains to environmental changes. We explore structure and dynamics of polystyrene sulfonic acid (PSSH) and salt (PSSNa) as a well-known polyelectrolyte in solution with low to high ion concentration (H+ and NaCl). The concentration of PE is well below the overlap concentration to examine the single chain regime. For single PE chains a transition from coils to globules is observed. Moreover, at some conditions ion condensation leads to pearl necklace conformation.
To elucidate the structure and form factor of PSSH SAXS and SANS (MLZ) measurements were conducted. Their combined analysis performed over a large Q-range allows us to examine the NaCl contribution and determine the details of intrachain structure.
NSE experiment (ILL) clearly shows change of polyelectrolyte dynamics as a function of salt concentration. Analysis of relaxation dynamics shows a change from a rigid body behavior (collapsed chains) to Zimm like dynamics as expected for strongly screened flexible polymer chains. The effect is temperature dependent.

Primary authors: BUVALAIA, Ekaterina; KRUTEVA, Margarita; Dr BIEHL, Ralf (JCNS)

Co-authors: FÖRSTER, Stephan (Forschungszentrum Jülich); RADULESCU, Aurel (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ); Dr HOFFMANN, Ingo (Institut Laue-Langevin)

Presenter: BUVALAIA, Ekaterina

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

Contribution ID: **159** Type: **Poster**

Neutron Depth Profiling at the PGAA facility of MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe profiles of lithium, nitrogen, boron, helium and several additional light elements concentration in different host materials. The N4DP experiment is located at the Prompt Gamma Activation Analysis (PGAA) facility of Heinz Maier-Leibnitz Zentrum (MLZ), which provides a cold neutron flux up to $5 \times 10^{10}\,\mathrm{s^{-1}cm^{-2}}$. When a neutron is captured by a ^{6}Li nucleus, the system emits an alpha particle at a well-defined energy. The loss of the charged particle traveling through the host material is related to the depth of origin at a resolution level up to a few ten nanometers.

After a short introduction to the existing N4DP facility, we will present the status of the ongoing upgrade towards its full functionality to study the lithium-ion concentration gradient in energy storage systems, i.e. Li-ion batteries. Here, NDP reveals new insights into the evolution of the lithium accumulation in different silicon-graphite anode compositions. The evolution of immobilized lithium could directly be measured, which is one of the main causes of battery lifetime limitation. This project is supported by the BMBF, Contract No. 05K19WO8.

Primary author: NEAGU, Robert

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Presenter: NEAGU, Robert

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **160** Type: **Talk**

On the Determination of Residual Stresses in AM Lattice Structures

Tuesday, December 8, 2020 1:40 PM (25 minutes)

The determination of residual stresses becomes more complicated with increasing complexity of the structures investigated. Unlike most of the fabrication techniques, laser powder bed fusion allows the production of lattice structures without any additional manufacturing step. These lattice structures consist of thin struts and are thus susceptible to internal stress-induced deformation. In the best case, internal stresses remain in the structures as residual stress. The determination of the residual stress in lattice structures through non-destructive neutron diffraction is described in this work. In the case of lattice structures, we show how to overcome two formidable difficulties: a) the proper alignment of the filigree structures within the neutron beam; b) the proper determination of the RS field in a representative part of the structure. The magnitude and the direction of residual stress are discussed. The residual stress in the strut was found to be uniaxial and to follow the orientation of the strut, while the residual stress in the knots is more hydrostatic. We show that strain measurements in at least seven independent directions are necessary for the estimation of the principal stress directions. The measurement directions should be chosen according to sample geometry and an informed choice on the possible strain field. Indeed, we finally show that if the most prominent direction is not measured, the error in the calculated stress magnitude increases considerably.

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Presenter: Dr FRITSCH, Tobias (Bundesanstalt für Materialforschung und -prüfung)

Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **161** Type: **Poster**

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

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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 RSA II (tangential/radial) etc.

Primary author: PIPICH, Vitaliy

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Presenter: PIPICH, Vitaliy

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **162** Type: **Poster**

Sample Environment at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

We report on the newest development of sample environment at MLZ

Primary authors: PETERS, Juergen; Dr WEBER, Alexander (Forschungszentrum Jülich GmbH)

Presenter: Dr WEBER, Alexander (Forschungszentrum Jülich GmbH)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **163** Type: **Poster**

Following the interface formation during sputter deposition on perovskite films

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Perovskite solar cells (PSCs) are promising for future and sustainable power production because they can be processed via up-scalable industrial deposition techniques such as printing or spray casting. Sputtering is a common technique for large scale metal electrode deposition. Understanding and controlling the interface formation during the sputtering process on perovskite is therefore important towards large-scale production of PSCs. In the present study, we sputtered gold on methylammonium-lead-iodide perovskite thin films. During the sputter deposition, we performed in-situ grazing-incidence small-angle X-ray scattering (GISAXS) to gain insight into the detailed steps of aggregation and growth of the sputtered metal layer. Thereby, GISAXS offers a way to gain information about the time evolution during the crucial steps of interface formation. Interestingly, the layer formation kinetics during sputtering are found to be very different for two samples of different surface roughnesses, the perovskite surface morphology seems to influence gold aggregation. On the smooth surface aggregates form of a certain size and spacing at first, which grow and merge until a closed layer is formed eventually. In contrast, the rougher surface seems to cause a broader size distribution of the gold seeds.

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

Presenter: REB, Lennart (TUM E13)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **164** Type: **Talk**

Towards Reflectivity profile inversion through Artificial Neural Networks

Thursday, December 10, 2020 4:30 PM (15 minutes)

The goal of Specular Neutron and X-ray Reflectometry is to infer materials Scattering Length Density (SLD) profiles from experimental reflectivity curves. This talk will focus on describing an original approach to the ill-posed non-invertible problem which involves the use of Artificial Neural Networks (ANN). In particular, the numerical experiments to be described deal with large data sets of simulated reflectivity curves and SLD profiles, whose aim is to assess the applicability of Data Science and Machine Learning technology to the analysis of data generated at large scale facilities. In fact, under certain circumstances, properly trained Deep Neural Networks are capable of correctly recovering plausible SLD profiles when presented with never-seen-before simulated reflectivity curves. A proper inclusion of such an approach within current data workflows would be able to offer two main advantages over traditional fitting methods when dealing with real experiments, namely, 1. no prior assumptions about the sample physical model are required and 2. the times-to-solution could be shrank by orders of magnitude, enabling faster batch analyses for large datasets.

Primary author: CARMONA LOAIZA, Juan Manuel (Scientific Computing Group; JCNS am MLZ; FZ-Jülich)

Presenter: CARMONA LOAIZA, Juan Manuel (Scientific Computing Group; JCNS am MLZ; FZ-Jülich)

Session Classification: DN2020: Digitalization and Machine Learning

Track Classification: DN: Digitalization and Machine Learning

Contribution ID: **165** Type: **Invited talk**

Development of novel Co-base superalloys for turbine applications by advanced characterization techniques

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Superalloys are key materials for energy conversion in jet engines, rockets or power plants. For more than 60 years, Ni-based superalloys are in use. Due to their unique two-phase microstructure, they retain their strength up to 70% of their melting temperature. In 2006, a new, ternary Co3(Al,W) compound was discovered that enabled the development of Co-based superalloys with similar microstructures than the conventional Ni-based superalloys.
In the following years, we developed compositionally complex Co-based superalloys with significantly improved properties starting from the simple ternary Co-Al-W alloys. In this talk, it will be shown how various advanced characterization techniques, such as in-situ high temperature neutron scattering with neutron diffraction at the beamline SPODI and Small-Angle Neutron Scattering at SANS-1 Together with Transmission Electron Microscopy and Atom Probe Tomography helped to understand the observed microstructures and the resulting mechanical properties. It was found that the matrix is under tension and the precipitates under compression due to a positive lattice misfit between both phases of up to 0.8%, which is larger compared to conventional Ni-based superalloys. Additionally, the volume fraction of the intermetallic precipitate phase is exceptionally high (up to 70%). These findings were essential to develop polycrystalline Co-based wrought alloys that show enhanced creep properties compared to conventional Ni-based wrought alloys.

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Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **166** Type: **Talk**

MIEZEFOC

Tuesday, December 8, 2020 5:35 PM (25 minutes)

Neutrons are ideal probes to study static and dynamic properties of magnetic materials and materials containing heavy and light elements. With the increasing interest in studying slow processes at large spatial scales for example i) in diffusion processes in soft matter samples and ii) the spin dynamics near quantum and thermal phase transitions it is important to develop instrumentation with very higher energy resolution down to the neV regime. TAS- or ToF-spectrometers are not suitable to achieve such high energy resolutions because of the gigantic loss of intensity involved in the selection of the small energy bands. An elegant solution to circumvent the intensity problem is the use of the Larmor precession of neutrons. Despite the significant progress made with Larmor precession techniques, it is still difficult to investigate small samples and samples under extreme conditions such as high pressure and large magnetic fields due to the small intensity. We present a new MIEZE concept using focusing optics before and within the MIEZE setup that allows the illumination of small samples i.e. volumes of a few mm^3. The major advantages are an increase of the intensity at the sample position and a strong decrease of the background because only the sample is illuminated and not the sample environment. Thus, the signal-to-background ratio can be strongly reduced.

Primary authors: GEORGII, Robert; Prof. BÖNI, Peter; HERB, Christoph (TUM)

Presenter: HERB, Christoph (TUM)

Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **167** Type: **Talk**

Influence of salt on oppositely charged Polyelectrolyte/Surfactant mixtures: A comparing neutron reflectometry and surface tension study

Thursday, December 10, 2020 1:45 PM (15 minutes)

The surface properties of oppositely charged polyelectrolyte/surfactant mixtures play an important role in colloidal dispersions (foams, emulsions) e.g. for cosmetics, cleaning products and in food technology.
Extensive research on such mixtures was already performed with the focus on different polyelectrolytes as well as surfactants. However, the influence of the ionic strength is still unclear.
This work focuses on the influence of added salt (NaBr or LiBr depending on the polyelectrolyte counterion) on the adsorption behaviour of mixtures of the anionic polyelectrolyte NaPSS or $sPSO_2$-220 with the cationic C_{14}TAB. Therefore, surface tension and neutron reflectometry (NR) measurements were performed with a fixed C_{14}TAB concentration and a variable polyelectrolyte concentration at different salt concentrations (10^{-4}, 10^{-3}, 10^{-2} M).
For NaPSS, NaBr reduces the surface tension over the whole studied polyelectrolyte concentration range (10^{-5} –10^{-3} monoM) and broadens the seen increase of surface tension at the bulk stoichiometric mixing point (BSMP). The surface excess of both components –detected by neutron reflectometry –correlates quite well with these finding. In contrast, LiBr reduces the surface tension of $sPSO_2$-220 only above the BSMP. Here, the finding of NR are not matching the surface tension results. Possible reason such as structural differences of the polyelectrolytes or sensitivity of measurements will be discussed.

Primary authors: BRAUN, Larissa; Prof. VON KLITZING, Regine (TU Darmstadt)

Presenter: BRAUN, Larissa

Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

Contribution ID: **168** Type: **Poster**

The small-angle scattering instrument SANS-1 at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

We present the features of the instrument SANS-1, a joint project of TUM and HZG [1]. SANS-1 features two velocity selectors with 10% and 6% $\Delta\lambda/\lambda$ and a fast TISANE 14-window double chopper, allowing efficiently tuning flux, resolution, duty cycle and frame overlap, including time resolved measurements with repetition rates up to 10 kHz. The polarization analysis option combines a compensated MEOP and an integrated RF-flipper.
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 ~40° on an array of single ^{3}He tubes, where a standard $\cos^3$ solid angle correction is no longer valid. SANS-1 features a flexible, spacious sample stage equipped with a heavy-duty 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 [2] and a dedicated HF-coil system for nanomagnetism/hyperthermia [3].
We show selected highlights and present our current developments, e.g. a high temperature furnace that works as an insert for the 5T magnet and a future high magnetic field project.

[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 Hyperthermia

Primary authors: MUEHLBAUER, Sebastian; VAGIAS, Apostolos (FRM2 / TUM); BUSCH, Sebastian (GEMS at MLZ, HZG); HEINEMANN, Andre; WILHELM, Andreas

Presenter: MUEHLBAUER, Sebastian

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **169** Type: **Poster**

Nested Optic for Neutron Focusing

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The investigation of small samples by neutron scattering is usually very time consuming due to the low available neutron flux density of neutron beams and small signals from the sample. Originally, neutron guides have been used to transport neutrons over large distances to make room for additional beamlines and for improving the signal-to-noise ratio. While being originally proposed to reduce the number of reflections and therefore the losses, elliptic neutron guides are enjoying an increasing popularity also for focusing neutron beams. However, elliptic guides do not image objects properly due to very strong coma aberrations which should be avoided. In order to overcome the aberrations, we propose using nested arrays of short elliptic mirrors.
In our contribution, we report on the investigation of a nested mirror optic at the beamline MIRA. The key properties of the optic are a large brilliance transfer of approximately 75% and the possibility of adjusting the beam size and the divergence of the neutron beam at the sample position by apertures placed before the nested mirror optic. Therefore, no beam shaping devices are required close to the sample position thus reducing the background significantly. Nested mirrors will also be particularly useful for the efficient extraction of neutrons from highly brilliant moderators such as at the ESS, because the common illumination losses associated with using neutron guides are avoided.

Primary author: HERB, Christoph (TUM)

Co-authors: GEORGII, Robert; BÖNI, Peter (Technische Universität München)

Presenter: HERB, Christoph (TUM)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **170** Type: **Talk**

Lithium Quantification in Lithium-Ion Batteries Using Operando Neutron Depth Profiling

Tuesday, December 8, 2020 5:35 PM (25 minutes)

Commercial Lithium-Ion Battery (LIB) cells are mostly based on graphite as anode material. During the first inter¬calation of Li into graphite, the electrolyte gets reduced at the anode, forming a nm-thick surface layer, the so-called solid electrolyte interphase (SEI). The SEI stops further electrolyte reduction but consumes Li during its formation. Neutron depth profiling (NDP) is a non-destructive technique and a suitable tool to measure Li concentrations as a function of depth. When irradiating the sample with a cold neutron beam, 6Li nuclides emit charged particles after neutron capture. The residual energy and the signal rate of the emitted 3H particles are correlated to depth and amount of Li. Thus, SEI growth and Li (de)intercalation in graphite anodes can be studied up to a depth of ca. 30 µm. Here, we present operando NDP data for the first charge/discharge cycle of a graphite anode vs. a LiFePO4 cathode, using a custom-designed coin cell casing with 0.5 mm diameter holes which are sealed with a 7.5 µm Kapton window. We will demonstrate that the cycling performance of the operando cell is comparable to a standard laboratory cell, show that it was possible to quantitatively track the Li concentration across the graphite electrode during cycling, and thus to correlate the amount of Li in the SEI layer with the first cycle irreversible capacity.1

1 Linsenmann, Trunk, Rapp, Werner, Gernhäuser, Gilles, Märkisch, Revay, Gasteiger, J. Elec. Soc. 167 (2020) 100554.

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Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **171** Type: **Poster**

FLUKA and MCNP simulation benchmark for neutron yield measurement in HBS project

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The High Brilliance Neutron Source (HBS) project was initiated at the Jülich Centre for Neutron Science of the Forschungszentrum Jülich (JCNS). This project aims to develop an accelerator-driven pulsed neutron source operating at low energy (below the spallation threshold) with high current ion beams (~100 mA) and optimized to deliver high brilliance neutron beams to a variety of neutron instruments.

In the framework of the HBS-project the neutron production in beryllium, vanadium and tantalum targets irradiated with protons of various energies (22, 27, 33 and 42 MeV) delivered by JULIC (Juelich Light Ion Cyclotron) was investigated. The neutron yield was determined via gamma-ray spectrometry measuring the count rate of 2.23 MeV prompt gamma-line of hydrogen induced by thermal neutron capture in the polyethylene moderator surrounding the target. For calibration, measurement with an AmBe source of well-known neutron emission was carried out. Corrections for neutrons escaping the moderator as well as for the spatial extension of the 2.23 MeV -gamma source inside the moderator were numerically performed using the Monte Carlo codes FLUKA and MCNP6.

In this work, the results of the simulations obtained with FLUKA and MCNP6 including the neutron yields of the targets and, the neutron and gamma correction factors to assess to the experimental neutron yields are presented and discussed. Finally, the simulated neutron yields are compared with the experimental neutron yields.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **172** Type: **Poster**

Covid-19 related research opportunities at the MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The Covid-19 pandemic is a global challenge with unprecedented individual health, societal and economic impact. Scientific research is needed in many fields in order to find solutions for these new challenges. This conference contribution sheds light on how neutrons can contribute to this endeavor. It especially addresses what research options are available at the MLZ for COVID-19 research. Of course, there is a priority set on the proposals handed in which are related to COVID-19 research. They can be sent in any time and will be approved in a very short time.

Many neutron instruments at the MLZ may contribute to COVID-19 related research in the future. And this is not only with respect to health and micro-biological aspects. Also materials research is needed for better masks or reflectometry for better surfaces where the corona virus cannot stick to or is quickly demolished.

As an example a contrast matching Small Angle Neutron Scattering binding study between nsp10 and nsp16 is proposed which at the moment suffers from a low binding affinity of the two viral proteins.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

Contribution ID: **173** Type: **Talk**

Revealing Anion Order in Holmium Hydride Oxide HoHO by Neutron Diffraction

Thursday, December 10, 2020 4:30 PM (15 minutes)

Heteroanionic hydrides are an emerging class of compounds with representatives showing ionic conductivity [1] or catalytic activity [2]. For holmium hydride oxide HoHO, the disordered CaF2 type structure was assigned and confirmed by powder neutron diffraction [2]. However, the analysis showed a deviation from the 1:1:1 composition: REH2+xO1-x. This demands the occupation of either octahedral interstices (H-rich) or the formation of defects (O-rich compound) and the differentiation and quantification of these species (H, O, voids) requests the combination of different methods. As the anionic ordering influences the ionic conductivity substantially [3], we conducted neutron diffraction measurements on both HoHO and the deuteride HoDO.

In contrast to the previous reports, both compounds crystallize in an ordered CaF2 substructure with space group F-43m (Heusler-LiAlSi type; a(HoHO) = 5.27550(13) Å, a(HoDO) = 5.27394(8) Å) with no significant underoccupation, mixing of sites, or occupation of the octahedral interstice. They are the first ionic substances to crystallize in this structure type, which is usually observed for metallic half-Heusler phases. Furthermore, HoHO shows an unusual resistivity towards air, as it decomposes only above 600 K, independent of O2 in the atmosphere.

1 K. Fukui et al., Nat. Commun. 2019, 10, 2578.

2 H. Yamashita et al., J. Am. Chem. Soc. 2018, 140, 11170.

3 H. Ubukata et al., Chem. Mat. 2019, 31, 7360.

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Session Classification: DN2020: Materials

Track Classification: DN: Materials

Contribution ID: **174** Type: **Talk**

SKADI: Small-Angle Neutron Scattering at ESS

Thursday, December 10, 2020 1:30 PM (15 minutes)

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] This contribution will detail the current construction status of SKADI. In addition, further practical requirements on components such as the sample area will 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 $8{\cdot}10^8$ n/s cm2 at sample position, which will make it the world SANS instrument in brilliance.
In addition to complex sample environments SKADI will also feature a newly developed detector system, SoNDe, developed within the EU Horizon2020 framework. [2]
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 in-situ measurements with custom made sample environments to provide “real-world” conditions.
[1] JAKSCH, S., et al. NIMA, 2014, 762, S. 22-30.
[2] JAKSCH, S., et al. Proceedings of the International Conference on Neutron Optics (NOP2017). 2018. S. 011019.

Primary authors: JAKSCH, Sebastian (Physicist); FRIELINGHAUS, Henrich (JCNS); Dr HANSLIK, Romuald (Forschungszentrum Jülich GmbH, ZEA-1); Mr KOZIELEWSKI, Tadeusz (Forschungszentrum Jülich GmbH, JCNS); DESERT, Sylvain (CEA Saclay - LLB); CHENNEVIERE, Alexis (Laboratoire Léon Brillouin)

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Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

Contribution ID: **175** Type: **Poster**

The SoNDe high-flux neutron detector

Wednesday, December 9, 2020 5:40 PM (20 minutes)

New high-flux and high-brilliance neutron sources demand a higher count-rate capability in neutron 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 the available 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 a modular and scalable solution that can also be used in other instruments or different contexts, 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

- Possible 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 cm x 5 cm) were measured under primary beam conditions at neutron scattering experiments. Combined with the high area coverage of the square modules and the high efficiency of the scintillator this allows to use high flux neutron sources to capacity.

[1] JAKSCH, S., et al. Proceedings of the International Conference on Neutron Optics (NOP2017). 2018. S. 011019.
[2] JAKSCH, S., et al. Cumulative Reports of the SoNDe Project July 2017. arXiv preprint arXiv:1707.08679, 2017.

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Presenter: JAKSCH, Sebastian (Physicist)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **176** Type: **Poster**

Magnetic dynamics in the single-domain state of the cubic helimagnet ZnCr2Se4

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Anisotropic low-temperature properties of the cubic helimagnet ZnCr₂Se₄ in the single-domain spin-spiral state are investigated by a combination of neutron scattering, thermal conductivity,and dilatometry measurements. In an applied magnetic field, neutron spectroscopy shows a complex and nonmonotonic evolution of the spin-wave spectrum across the quantum-critical point that separates the spin-spiral phase from the field-polarized ferromagnetic phase at high fields. A tiny spin gap of the pseudo-Goldstone magnon mode, observed at wave vectors that are structurally equivalent but orthogonal to the propagation vector of the spin helix, vanishes at this quantum critical point, restoring the cubic symmetry in the magnetic subsystem. The anisotropy imposed by the spin helix has only a minor influence on the lattice structure and sound velocity, but has a much stronger effect on the heat conductivities measured parallel and perpendicular to the magnetic propagation vector. Anisotropic thermal transport is magnetic in origin and highly sensitive to an external magnetic field. We also report long-time thermal relaxation phenomena, revealed by capacitive dilatometry, which are due to magnetic domain motion related to the destruction of the single-domain magnetic state. Our results can be generalized to a broad class of helimagnetic materials in which a discrete lattice symmetry is spontaneously broken by the magnetic order.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

Contribution ID: **177** Type: **Poster**

Structured graphite anodes for Li-ion batteries

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Laser structured electrodes for Li-ion batteries have been reported as a promising approach for improvement of battery performance. The contact area between the electrolyte and active material in the electrode can be modified as a result of the three-dimensional structured electrode surface. The effective Li-ion diffusion pathways are shortened during the charging and discharging of the cell. Surface structuring can potentially reduce cell internal resistance, which has a positive impact on the battery performance at high C-rates. In this work, electrochemical properties of the laser structured and unstructured graphite anodes in fresh and aged NMC/C cells were studied. The aim was to examine cell performance at high C-rates. NMC/C pouch cells were studied via in-situ neutron diffraction, an important method for characterizing the structural changes before/after the intercalation of Li into graphite. It has been confirmed that the electrochemical performance of the laser structured electrodes has been improved and that there are no structural changes present in the active material caused by laser irradiation. These results bring many insights for our future work in the area of structured 3D electrodes. One possibility to shorten the ion diffusion paths in the battery cells is by preparing the electrodes using additive manufacturing. This method offers many opportunities for innovative electrode and cell design, thanks to its high precision and diversity.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **178** Type: **Poster**

Microstructural characterization of European historical swords through neutron imaging

Wednesday, December 9, 2020 5:40 PM (20 minutes)

It is evident from several analyses performed on steel samples that the production of arms and armor used cutting edge technology of that time so a study of such artefacts can give fundamental details about the technological skills of a specific area or period. In order to correlate similar samples of a specific age or provenance, it is important to build trustworthy classification parameters. Neutron imaging techniques allow us to determine the morphology and microstructure of composite steel artefacts thus allowing us to characterize the composition, the steel quality, the welds and thermal treatment.
We started a systematic study to characterize the production methods of European swords from the early Middle Ages to the 17th century. On this purpose we started analyzing three swords of great importance now belonging to the Bayerisches Nationalmuseum.
-Longsword, produced in Tyrol in the late 15th century, inv. W872.
-Hunting sword, produced by M. Diefstetter (bladesmith), Munich, c. 1550 (blade) (grip), inv. W579.
-Sword, produced in Northern Italy, possibly Milan, c. 1560, inv. W587.
White beam tomography allowed detecting the presence of several features in the bulk of the blades as multilayered structures, cracks and defects, and determining the width and the shape of the martensitic hardened edges. Energy selective analysis allowed determining details of the steel composition and microstructure as well as mapping the different low and high carbon areas.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Heritage Science

Contribution ID: **179** Type: **Poster**

Influence of salt (NaCl) on structure and dynamics of phospholipid membranes

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Phospholipid membranes are the construction material of cell membranes and solutions of phospholipid vesicles find a range of applications in technical, medical and biological applications.
We previously showed the structure (neutron reflectometry, GISANS) and the dynamic behavior (GINSES) of L-α-phosphatidylcholine (SoyPC) phospholipid membranes. [1,2] We established a multi-lamellar structure as well as a surface mode, attributed to transient waves in the membranes.
We extended those studies to investigate the influence salt (NaCl) concentration in the system, both in order to ascertain the difference between previously investigated strongly hydrophobic additives as well as better represent an in-vivo biological membrane.
Two features of the membrane system were revealed: (1) The thickening of the membrane layers as reported by SAXS measurements is due to an enriched counter-ion area close to the head group of the phospholipid membranes, and not, as for hydrophobic molecules an actual swelling of the membrane. (2) The in-plane dynamics of the membranes is enhanced by the addition of NaCl, while retaining the previously reported surface mode.
Those features can play an important role in the understanding of membrane functions, such as the formation of ion channels, and thus their biological function on a fundamental level.
[1] S. Jaksch, H. Frielinghaus et al, Phys. Rev. E 91(2), 2015, 022716.
[2] S. Jaksch, H. Frielinghaus et al, Scientific Reports 7(1), 2017, 4417.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

Contribution ID: **180** Type: **Poster**

In-situ RheoSAXS: Relating Nanostructure to Macroscopic Properties Using A Laboratory Setup

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Material research in all its complexity continuously calls for new analysis solutions to solve sophisticated issues in one go.
Rheology deals with the flow and deformation of matter. Applying shear force to a material can result in orientation or crystallization. With small-angle X-ray scattering (SAXS) structural parameters of nanomaterials such as size, shape, inner structure, and orientation can be determined. Relating the nanostructure of a material to its macroscopic mechanical properties requires in-situ characterization techniques such as rheology combined with SAXS. RheoSAXS experiments have so far only been conducted at synchrotron beam lines, mainly due to the insufficient X-ray flux of laboratory X-ray sources and the lack of a dedicated RheoSAXS laboratory setup.
In this contribution we present a novel experimental setup for performing combined RheoSAXS studies with the SAXSpoint 2.0 laboratory SAXS system.
The integrated RheoSAXS sample stage enables temperature-controlled rheological experiments with in-situ determination of shear-induced structural changes of nanostructured materials on a nanoscopic length scale (from approx. 1 nm to 200 nm) by SAXS. The RheoSAXS module includes a rheological sample compartment which is integrated in the evacuated SAXS measurement chamber. The rheometer measuring head comprises a high-precision air-bearing motor which holds and controls the rheological scattering measuring system in the SAXS instrument chamber.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **181** Type: **Talk**

Polymorphic phase transition in liquid and supercritical carbon dioxide

Thursday, December 10, 2020 4:45 PM (15 minutes)

Thermal density fluctuations of supercritical (SC) CO2 were explored using small-angle neutron scattering (SANS) whose amplitude (susceptibility) and correlation length show the expected maximum at the Widom line. The susceptibility is in excellent agreement with the evaluated values on basis of mass density measurements. A surprising observation is droplet formation above the gas-liquid line and between 20 and 60 bar above the Widom line, the corresponding borderline identified as the Frenkel line. The droplets start to form spheres of constant radius of about 45 Å and transform into rods and globules at higher pressure. The droplet formation represents a liquid-liquid (polymorphic) phase transition of same composition but different number density, whose difference defines its order parameter. Polymorphism in CO2 is a new phenomena, it characterizes the gas-like to liquid-like transition in SC fluids and might be of particular interest for better understanding polymorphism, since CO2 represents a "simple"van der Waals liquid in contrast to water, which is the most widely studied liquid showing polymorphism in its supercooled state.

This work has been published in:
Phys. Rev. Lett. 120 (2018) 145701.
Scientific Reports (2020) 10:11861. doi.org/10.1038/s41598-020-68451-y.

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Session Classification: DN2020: Materials

Track Classification: DN: Materials

Contribution ID: **182** Type: **Poster**

Validating Molecular Dynamics Computer Simulations with Neutron Scattering Data

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron scattering data are usually evaluated by analytical models. Computer simulations, for example using the Molecular Dynamics (MD) technique, can give a description of the sample's structure and dynamics on the atomic scale. Using this information, neutron (and x-ray) diffraction and spectroscopy curves can be computed. The scattering data can then be used to validate the simulations and vice versa the simulations can be used to evaluate the scattering data. These evaluations are able to capture complicated structures (e.g., amorphous) and motions (e.g., non-Fickean diffusion).
In this contribution, we focus on the comparison of different exemplary simulations of solids and liquids to scattering data.
For the solids, the influence of different parameters of the simulation such as the size of the simulated box on diffraction patterns is evaluated and the accuracy of the computation results using the program SASSENA is discussed for neutron and x-ray diffraction.
In the case of liquids, the simulated structure and dynamics of water as a prototypical liquid is compared to scattering data and other literature values like the diffusion coefficient. Different force fields are investigated and the influence of their base parameters is studied.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Digitalization and Machine Learning

Contribution ID: **183** Type: **Poster**

Nondestructive determination of Li concentration and distribution in prismatic Li-ion battery

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Li-ion batteries' (LIBs) popularity is a result of their outstanding characteristic, in particular high capacity, long lifetime, no memory effect. Among different form factors, the prismatic cells are mostly used for small electronics, but they also become an attractive option for e-mobility applications in the latest years. Among various experimental tools, the powder diffraction has been a proven one for studies of Li-ion batteries. In particular, synchrotron and neutron radiations enable non-destructive probe of structure for LIB components and their constituents under real and non-ambient operating conditions. 2D Li distribution inside the prismatic cell for the anode and the cathode can be traced by utilizing high-energy X-ray diffraction. Employing neutron diffraction with a thermal monochromatic neutron beam both ex-situ and in-situ/operando studies of prismatic LIBs are possible as it was recently reported.
In the current contribution, a fresh and electrochemically aged commercial prismatic LIBs used in the iPhone 6 were inspected by both X-ray diffraction radiography and neutron powder diffraction. Neutron diffraction allowed the evaluation of the overall structural changes of cell constituencies in the prismatic LIB, which were correlated to electrochemical treatment, where the changes of 2D Li distribution were determined with high energy X-ray diffraction.

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Presenter: BARAN, Volodymyr

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Structure Research

Contribution ID: **184** Type: **Plenary talk**

Advances in the study of stimuli-responsive core-shell microgel particles

Thursday, December 10, 2020 9:30 AM (30 minutes)

The synthesis of complex microgel architectures triggers the necessity of structural characterization. Small angle neutron scattering (SANS) is well suited for this purpose. SANS is capable of simultaneously measuring both average particle sizes and polydispersity, as well as the local structure of colloidal gels. SANS and isotopic substitution may reveal the distribution of monomers within particles, as for example in core-shell microgels having one monomer deuterated. It is the ultimate goal of our approach extracting radial density profiles of the microgel network. The talk will discuss modelling approaches to analyse SANS data from such systems. Contrast matching through the solvent and employing isotopic substitution of either shell or core monomers enables studying the monomers selectively in SANS. One should note that deuteration causes differences in swelling, as published by us for p(NIPMAM) [1], but its impact remains negligible far from the volume phase transition temprature. We add that although SANS is not the only technique to observe microgels [2], it is indeed very powerful due to the possibilities of deuteration allowing differentiating core and shell polymer, in bulk suspensions [3].

[1] Cors M, Wiehemeier L, Oberdisse J, Hellweg T (2019). Polymers 11(4):620

[2] Bergmann S, Wrede O, Huser T, Hellweg T (2018). Phys Chem Chem Phys 20:5074

[3] Cors M, Wrede O, Wiehemeier L, Feoktystov A, Cousin F, Hellweg T, Oberdisse J (2019). Sci Rep 9(1).

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Session Classification: DN2020: Plenary talks

Track Classification: DN: Plenary talks

Contribution ID: **185** Type: **Poster**

Monte Carlo simulation and optimization for the micro-channel target of the HBS project

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The High Brilliance Neutron Source (HBS) project was initiated at the Jülich Centre for Neutron Science of the Forschungszentrum Jülich (JCNS). It aims to develop a medium neutron source facility based on a linear accelerator, scalable up to 70 MeV proton energy and optimized to deliver high brilliance neutron beams to a variety of neutron instruments. In the framework of this project a compact micro channel target was proposed for the powerful high-flux and compact, accelerator-driven neutron sources (CANS). Based on earlier simulations concerning fluid dynamics and structural mechanics, a preliminary design was developed. Due to the required compactness, heat dissipation and mechanical stability are the factors limiting the total neutron yield of the target. In order to find a compromise solution between high neutron yield and mechanical stability, the energy desposition as well as neutron and proton spectrum in different geometric parameters of the micro-channel target were performed with the Monte Carlo simulation code FLUKA. The details of the simulation and optimization will be presented at the workshop.

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Presenter: Ms DING, Qi

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **186** Type: **Poster**

Towards Polarization Analysis for TOPAS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The thermal time-of-flight spectrometer TOPAS has been constructed by the Jülich Centre for Neutron scattering (JCNS) and is now awaiting neutrons in the neutron guide hall east at the Heinz Maier-Leibnitz Zentrum (MLZ). The instrument design provides wide-angle polarization analysis (PA) for the thermal energy range. While recently other thermal time-of-flight spectrometers with PA have been taken into operation, TOPAS relies on novel and unique polarization devices. To gain experience, individual components went through thorough testing on other instruments. We will present tests of the TOPAS polarizer on POLI, which features continuous spin-exchange optical pumping (SEOP). Already in this test, the performance for neutron energy up to beyond 100 meV was excellent and lead to development of dedicated equipment for POLI. Tests of the wide-angle XYZ analysis have been performed during the last year of operation of the NEAT spectrometer at the HZB. Finally, we report on the progress with the installation of the instrument in the guide hall east.

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Presenter: FRANZ, Christian

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **187** Type: **Talk**

Multimodal Imaging using Neutrons and Gammas at the NECTAR Instrument

Tuesday, December 8, 2020 1:40 PM (25 minutes)

NECTAR is a unique beam-line with access to fission neutrons for non-destructive inspection of large and dense objects, where thermal neutrons or X-rays face limitations due to their comparatively low penetration. With the production of fission neutrons at the instrument, as well as neutrons interacting with beamline geometry, such as the collimator, gamma rays are inevitably produced in the same process. Furthermore, these gamma rays are highly directional due to their constraint to the same beam-line geometry and come with similar divergence as the neutrons. While difficult to shield, it is possible to utilize them by using gamma sensitive scintillator screens in place of the neutron scintillators, viewed by the same camera and swapped-out in-situ.
Here we present the advantages of combining the information gained from neutron imaging in conjunction with gamma imaging at the NECTAR beam-line, providing a unique probe with unparalleled isotope identification capabilities.

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Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **188** Type: **Poster**

Multimodal Imaging from meV to MeV Neutrons combined with Gamma Imaging at the NECTAR Instrument

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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 advantages of combining the information gained from neutron imaging in conjunction with gamma imaging at the NECTAR beam-line, providing a unique probe with unparalleled isotope identification capabilities with examples provided for archaeology, batteries, industry components and scintillator materials. Furthermore, we provide an update on the recent progress at NECTAR, with upgraded capabilities, such as the addition of gamma and single event-mode imaging.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **189** Type: **Talk**

T-odd effects in the binary fission of uranium induced by polarized neutrons

Tuesday, December 8, 2020 2:05 PM (25 minutes)

T-odd effects in the fission of heavy nuclei have been extensively studied during more than a decade in order to study the dynamics of the process. A collaboration of Russian and European institutes discovered the effects in the ternary fission in a series of experiments performed at the ILL reactor [1-2] and the effects were carefully measured for a number of fissioning nuclei. The analogous effects for gammas and neutrons in fission of 235U and 233U was also measured [2-5] after the observation of T-odd effects for ternary particles accompanying the reaction 235U(n,f) induced by cold polarized neutrons. All experiments up to now were performed with cold polarized neutrons, which suggests a mixture of several spin states of the compound nucleus, the relative contributions of which are not well known. The measurements of gamma and neutron asymmetries in an isolated resonance of uranium is important in order to get "clean"data. The present work describes a number of our team's measurements that include the results of T-odd effects in the fission of uranium isotopes by polarized neutrons with different energies at the POLI facility and the MEPHISTO beamline of the FRM2 reactor in Garching.
[1] P.Jesinger et al., Phys.At.Nucl. 62, 1608 (1999)
[2] Y.Kopatch et. al., EPJ Web of Conf. 169, 00010 (2018)
[3] G.Danilyan et al., Phys.At.Nucl. 72, 1812 (2009)
[4] G.Danilyan et al., Phys. At. Nucl. 74, 671 (2011)
[5] G.Danilyan et al., Phys.At.Nucl. 74, 671 (2011)

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Session Classification: MLZ Users 2020 - Nuclear, Particle, and Astrophysics

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **190** Type: **Poster**

MARIA –The high-intensity polarized neutron reflectometer of JCNS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

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) as a primary wavelength filter with 10% resolution. In combination with a Fermi-Chopper the wavelength resolution can be increased to 1% or 3%. The beam is optionally polarized by a double-reflecting super mirror and the elliptically focusing neutron guide increases the flux at the sample position thus 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), a UHV-chamber (10–10 mbar range) for the measurement of Oxide MBE samples and also with soft matter solid/liquid interface cells connected to a "sample robot"for automatic solvent contrast. Together with the 400 x 400 mm² position sensitive detector and a ^{3}He polarization spin filter based on Spin-Exchange Optical Pumping, the instrument is well equipped for investigating specular reflectivity and off-specular scattering from magnetic layered structures. Furthermore the GISANS option can be used to investigate lateral correlations in the nm range.
MARIA is a state of the art reflectometer that gives the opportunity to investigate reflectivity in a dynamic range of up to 7-8 orders of magnitude including off-specular scattering and GISANS. Furthermore the high intensity allows for kinetic measurements down to a few seconds over a dynamic range of 4 orders.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **191** Type: **Poster**

Thin film growth by Molecular Beam Epitaxy for MLZ users

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Molecular Beam Epitaxy (MBE) is a versatile tool to fabricate high quality and high purity epitaxial thin films. At MLZ, the Jülich Centre for Neutron Science (JCNS) runs an MBE system to provide samples for users who either do not have the expertise to prepare thin film samples for their neutron experiments and/or the equipment.

In other words: If you need thin film samples for your neutron experiments, let's discuss how we can prepare your samples!

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

Thin film samples which are sensitive to ambient conditions are first fabricated in the MBE system and then measured at the neutron reflectometer MARIA of JCNS utilizing a versatile small ultra high vacuum condition chamber.[1]
In our presentation we will present examples for high quality thin films like e.g. FeN, Fe_4N, $SrCoO_3$ or Nb/Al_2O_3(1-1 0 2) and link them to neutron experiments.

[1] A. Syed Mohd, S. Pütter, S. Mattauch, A. Koutsioubas, H. Schneider, A. Weber, and T. Brückel, Rev. Sci. Instrum., vol. 87, pp. 123909, 2016

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Quantum Phenomena

Contribution ID: **192** Type: **Poster**

DMPC-glycyrrhizin model membranes in the absence and presence of cholesterol: From small unilamellar vesicles to flat disc structures

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The saponin glycyrrhizin is the main sweet-tasting part of the liquorice root and is often used as a sweetener and emulsifier. It is known to interact strongly with cholesterol and has anti-viral activity. Using small, unilamellar lipid vesicle (SUV) as model membrane, we study the mixing properties of glycyrrhizin with the phospholipid 1,2-dimyristoyl-sn-glycero-phosphocholine (DMPC) by using small-angle neutron scattering (SANS). Due to the phase transition temperature of DMPC at $T_m \approx 24$ ℃, the fluid-like state (above T_m: 40 ℃) and the solid-like state (below T_m: 10 ℃) of the DMPC bilayers were studied. SANS measurements show that DMPC vesicles with and without cholesterol (10 mol%) generate a vesicle like form factor. The interaction of glycyrrhizin with the DMPC bilayer can be differentiated into three regimes which are based on the concentration of glycyrrhizin. Below 7 mol%, glycyrrhizin is incorporated into the bilayer (with and without cholesterol), respectively for both states of the bilayer. From 10 to 30 mol% aggregation occurs and above 30 mol% the form factor indicated the presence of smaller structures, for a solid-like state of the bilayer. In the presence of cholesterol, aggregation is observed not before 15 mol% glycyrrhizin and no nano discs are formed. For the membrane in the fluid-like state aggregation occurs up to 40 mol% glycyrrhizin. Beyond this value no aggregation can be observed. Small structures can only be found from 60 mol% onwards.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **193** Type: **Talk**

Aqueous foams stabilized by PNIPAM microgels: A SANS study

Tuesday, December 8, 2020 5:10 PM (25 minutes)

Probing the internal structure of macroscopic liquid foams, like their film thickness, is very difficult or even impossible with optical methods, since foams strongly scatter light in the visible range. To overcome this problem, small angle neutron scattering (SANS) can be used, as already demonstrated by Axelos et al. [1].
This contribution addresses foams stabilized by Poly-N isopropylacraylamide (PNIPAM) microgels. These foams are very stable at temperatures below the VPTT and can be destabilized on demand by increasing the temperature. The internal structure of these is investigated with SANS experiments, which allows for the thickness determination of foam films inside the foam.
Four microgels with varying cross-linker concentration were used to study the influence of particle stiffness on the foam film thickness. Furthermore, each foam was probed at three different heights inside of the foaming column, which corresponds to different times after the foam formation, to probe the evolution of film thickness over time.
These findings, combined with the knowledge about the mechanical properties of individual microgels, are used to explain the macroscopic foam properties, namely foamability and foam stability.

[1] M. Axelos and F. Boué, *Langmuir*, **2003**, 6598.

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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **194** Type: **Poster**

Field Dependence of Magnetic Disorder in Nanoparticles

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Being intrinsic to nanomaterials, disorder effects crucially determine the properties of magnetic nanoparticles, such as their heating performance [1-3]. However, despite the great technological relevance and fundamental importance, a quantitative interpretation of the three-dimensional magnetic configuration and the nanoscale distribution of spin disorder within magnetic nanoparticles remains a key challenge.
Here, I will present our recent studies on the intraparticle magnetization distribution in ferrite nanoparticles [4]. In contrast to the classical, static picture of a collinearly magnetized particle core with a shell of structurally and magnetically disordered surface spins, we establish a significant field dependence of the nanoparticle moment and demonstrate how magnetic order overcomes structural disorder. In our study, polarized SANS [5] extends the traditional macroscopic characterization by revealing the local magnetization response and allows us to quantitatively separate surface spin disorder from intraparticle disorder. Finally, we elucidate the intraparticle distribution of the spin disorder energy, giving indirect insight into the structural defect density in magnetic nanoparticles.

[1] P. Bender et al., J. Phys. Chem. C 122, 3068 (2018).
[2] A. Lak et al., Nano Lett. 18, 6856 (2018).
[3] A. Lappas et al., Phys. Rev. X 9, 041044 (2019).
[4] D. Zákutná et al., Phys. Rev. X 10, 031019 (2020).
[5] S. Mühlbauer et al., Rev. Mod. Phys. 91, 015004 (2019).

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

Contribution ID: **195** Type: **Poster**

NREX - neutron reflectometer with X-ray option

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The high resolution neutron/ X-ray contrast reflectometer NREX, operated by the Max Planck Institute for Solid State Research, is designed for the determination of structural and magnetic properties of surfaces, interfaces, and thin film systems.
The instrument is an angle-dispersive fixed-wavelength machine with a default wavelength of 4.28 Å. A horizontal focusing monochromator gives the possibility to switch between modes "high intensity/ relaxed resolution"and "high resolution/ reduced intensity"and provides a beam especially for small samples (down to 5×5 mm2 and below). A Beryllium filter attenuates higher order reflections. Transmittance supermirrors m = 3.5 with a polarizing efficiency of P>99% and high efficiency gradient RF field spin flippers are used for a full 4 spin channel polarization analysis.
The sample is aligned horizontally. By tilting the sample the incident angle is varied. The detector arm can move for GISANS horizontally as well as vertically for specular and diffuse scattering measurements. Neutrons are detected with a 20 x 20 cm^2 position sensitive or a pencil detector. An X-ray reflectometer can be mounted on the sample table orthogonal to the neutron beam. It allows for the in-situ characterization of sensitive soft matter samples and neutron/ X-ray contrast variation experiments.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **196** Type: **Talk**

Search for vacancies in concentrated solid-solution alloys

Tuesday, December 8, 2020 5:10 PM (25 minutes)

Concentrated solid solution alloys (CSA) with no principle alloying element but a single randomly populated crystal structure exhibit attractive material properties, e.g., high ductility at low temperatures or high irradiation resistance. To understand such phenomena in these alloys, often also named high-entropy alloys, assessment of atomic transport including formation and migration of vacancies is indispensable. Here results of positron annihilation lifetime spectroscopy (PALS) are reported to quantify the concentration of quenched-in thermal vacancies for CSAs with fcc structure after quenching from temperatures close to their onset of melting. This vacancy concentration decreases with increasing number of components. For alloys with 3 constituents in non-equimolar fractions (CrFeNi) vacancy concentrations in the 10^{-5} range were determined. However, for alloys with 4 (CoCrFeNi) and 5 constituents (CoCrFeMnNi, AlCoCrFeNi) a vacancy-specific positron lifetime was not detected. Thus, the concentration of quenched-in vacancies must be 10^{-6} or less. This indicates either a vanishingly small fraction of vacancies present at very high temperatures or generated vacancies are inherently unstable. For an unambiguous proof, in-situ positron studies during heating and cooling between room temperature and high temperatures are necessary. Such experiments are planned using a positron beam in the longstanding collaboration with Chr. Hugenschmidt (NEPOMUC beamline at FRM II).

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Session Classification: MLZ Users 2020 - Materials Science

Track Classification: UM: Materials Science

Contribution ID: **197** Type: **Poster**

Engineering of the thermal moderator for a Compact Accelerator driven Neutron Source (CANS)

Wednesday, December 9, 2020 5:40 PM (20 minutes)

In a CANS, different from a research reactor or a spallation source, the primary neutrons are produced inside a volume below 200 cm^3. One of the main requirements for a well-optimized research neutron source is to convert this compact fast neutron cloud into a compact thermal neutron cloud. There the geometry needs to be suitable for the extraction of neutron beams towards the instruments. In addition, the time structure of the pulsed proton beam impinging on the target is convoluted with the time constants of the moderation, absorption, and diffusion processes inside the moderator material.
In this presentation, we present simulations performed by exact MCNPx Monte-Carlo methods and approximated analytical diffusion-based models. We will show the effect of different moderator materials (hydrogen, deuterium, beryllium, and carbon based), dilution, poisoning, and combination of different materials inside the thermal moderator and with reflectors surrounding the thermal moderator on the peak flux and the time structure of the neutron beams delivered to a potential instrument.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **198** Type: **Poster**

Event-Mode Imaging for Improved Spatial Resolution in Fast Neutron Imaging

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Event-Mode Imaging is a method where the final image is obtained as a summation of individually acquired particle interactions. In fast neutron scintillators, scattering of the high energy neutrons generates recoil protons. Ionization by the protons leads to creation of visible light in the form of a cone. The low spatial resolution in fast neutron imaging results from blurring introduced by the cone shape emission of light with the spatial resolution roughly proportional to the thickness of the scintillation material. To overcome the problem of spatial locality, a center-of-mass method is used to find the most probable location of the spot for each neutron interaction, potentially allowing to increase spatial resolution and efficiency of the method.

Here we present a parametric study for event-based imaging to computationally obtain optimal parameters, such as the impact of noise, the size of the light spot, the deviations in the center-of-mass methodology and so on through simulations. This is done by random probabilistic sampling of pixels in a grayscale input image simulating the particle interaction and applying a Gaussian blur patch to the sampled pixel value with a kernel size to replicate the problem of low spatial resolution in the simulation. Furthermore, we present the initial results of data acquired using an event-based detector system with each event processed by the proposed methodology.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **199** Type: **Poster**

Neutron guides and Ni/Ti multilayer supermirror coatings by the FRM II Neutron Optics group

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The MLZ makes extensive use of modern neutron guides to transport and distribute the neutrons over large distances, which are installed and maintained by the neutron optics group. Adapted to the needs of the instruments with respect to wavelength distribution and angular dispersion the guide elements are coated by 58Ni or Ni/Ti supermirror coatings with m values up to 3.5 either procured externally or produced in our DC magnetron sputtering facility. The neutron optical properties of the individual mirror plates are verified with our neutron reflectometer TREFF. In the last year, a decent effort was made to improve the quality of the supermirrors produced by the neutron optics group in terms of reducing mechanical stress and increasing their reflectivity. For this purpose, experiments were conducted to optimize different parameters of the production process. The success of those experiments lead us to get supermirrors with better reflectivities and allowed us to explore the design and production of supermirrors with larger angle of total reflection beyond m=3.5, which was historically our limit. We present our in house neutron guide production and other service for the instruments.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **200** Type: **Talk**

How to properly #opendata?

Thursday, December 10, 2020 4:45 PM (15 minutes)

Within the last decade, neutron instrumentation improved in many ways. We are no longer presenting original datasets in consequence of drastic increase in the amount of taken data. Published figures depends on many independent parameters, like binning size, data reduction algorithms, instrumental corrections. It is clear that in order to to keep our data useful we need to change the ways how we treat them.

I will present you detailed process of opening neutron data, touching several topics:

1. Publishing raw data: open access repositories (like figshare) vs. facility repositories (data.ill.eu or SciCatProject)
2. Publishing evaluation scripts: keeping scripts accessible after hundreds of years, docker images for easy data evaluation.
3. Versioning and citability of your code: how to cite github projects, sharing code between community, dissemination of your research with open code approach.
4. Transformation of datasets to open education resources.
5. Data journals: future of data sharing.

Opening my research helped me to stay organized and expanded my collaboration network. I hope I will convince you for #opendata as well.

1: McKiernan, Erin (2020): Connections between open scholarship practices. figshare. Figure. https://doi.org/10.6084/m9.figshare.12592283.v2

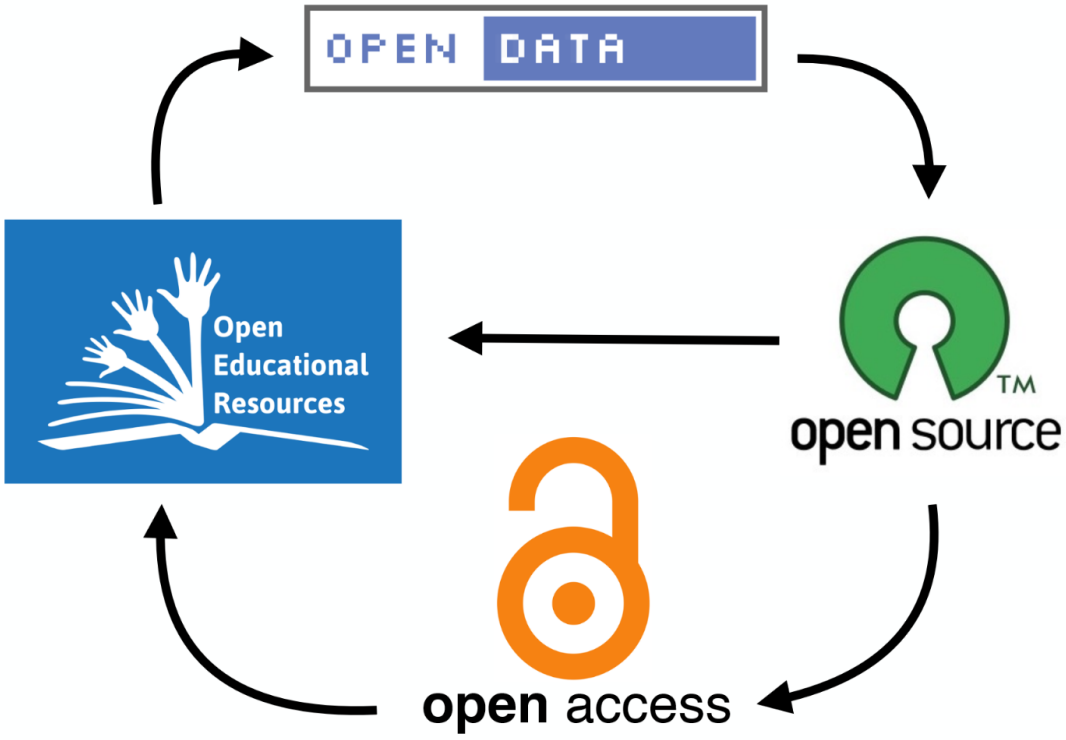

Figure 1: Open approaches interaction [1]

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Session Classification: DN2020: Digitalization and Machine Learning

Track Classification: DN: Digitalization and Machine Learning

Contribution ID: **201** Type: **Poster**

Establishing deuteration services for MLZ users at the JCNS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron scattering experiments involving soft matter materials often require specific contrast to observe different parts of the materials. In order to increase the availability of deuterium labelled materials, we are establishing deuteration support to MLZ users. At this state, we are focusing on a limited number of projects, but in the future, a proposal based deuteration service will be available in GhOST in combination with a proposal for neutron beamtime. Furthermore, the JCNS deuteration efforts are embedded in the LENS deuteration initiative, with the objective of providing in the future a source independent deuteration support together with ILL, ESS and ISIS.

Our main synthetic focus at JCNS-1 is in the area of polymer and organic chemistry. Anionic and controlled radical polymerization techniques allow the synthesis of e. g. polydienes, polyethylene oxide, polybutylene oxide polyacrylates and methycrylates with narrow molecular weight distributions for well-defined samples. The so obtained polymers can be functionalized afterwards to attach diverse functional groups or molecules. Organic techniques are used for the production of ionic liquids, surfactants, lipids, monomers and other compounds. The presentation summarizes the synthetic expertise available at JCNS-1 as well as outlines the planned process to establish the deuteration support. We are looking forward to answering your questions at our poster!

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **202** Type: **Talk**

Establishing deuteration services for MLZ users at the JCNS

Tuesday, December 8, 2020 3:50 PM (25 minutes)

Neutron scattering experiments involving soft matter materials often require specific contrast to observe different parts of the materials. In order to increase the availability of deuterium labelled materials, we are establishing deuteration support to MLZ users. At this state, we are focusing on a limited number of projects, but in the future, a proposal based deuteration service will be available in GhOST in combination with a proposal for neutron beamtime. Furthermore, the JCNS deuteration efforts are embedded in the LENS deuteration initiative, with the objective of providing in the future a source independent deuteration support together with ILL, ESS and ISIS.

Our main synthetic focus at JCNS-1 is in the area of polymer and organic chemistry. Anionic and controlled radical polymerization techniques allow the synthesis of e. g. polydienes, polyethylene oxide, polybutylene oxide polyacrylates and methycrylates with narrow molecular weight distributions for well-defined samples. The so obtained polymers can be functionalized afterwards to attach diverse functional groups or molecules. Organic techniques are used for the production of ionic liquids, surfactants, lipids, monomers and other compounds. The presentation summarizes the synthetic expertise available at JCNS-1 as well as outlines the planned process to establish the deuteration support.

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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **203** Type: **Poster**

Development of a Sample Environment for in-situ Dynamic Light Scattering in Combination with Small Angle Neutron Scattering for the Investigation of Soft Matter at the European Spallation Source

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The most brilliant and most powerful neutron source in the world, the European Spallation Source ESS, is currently built in Lund. In the scope of the project "FlexiProb"three modular sample environments for the investigation of soft matter samples to maximize the potential of the ESS with regard to the very high neutron flux are being developed.
These are sample environments for small angle neutron scattering (SANS) with *in-situ* dynamic light scattering (DLS), under gracing incidence (GISANS) developed at TU Munich and on free-standing liquid films and foams developed at TU Darmstadt. All sample environments are built on an universal carrier system to ensure a high repeatability and flexibility as well as a minimum switching time between different sample environments and SANS machines.
The *in-situ* DLS & SANS module developed in our subproject will provide additional control parameters, in particular the sample stability, during the SANS measurements. For that, the module allows the simultaneous measurement of SANS and DLS at two different scattering angles and instant evaluation of the sample sizes distribution. To accomodate for the high neutron flux at ESS, we developed a special sample holder suitable for the precise temperature control of about 40 samples.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **204** Type: **Poster**

Distortions and Superstructure in Inverse Perovskite Nitrides

Wednesday, December 9, 2020 5:40 PM (20 minutes)

We discovered nitrogen/defect ordering leading to elpasolite-type superstructures in inverse perovskites with the general composition (A3Nx)Tt (A = Ca, Sr, Ba; Tt = Si, Ge, Sn, Pb). Due to the large scattering length of nitrogen, neutron powder diffraction is crucial when it comes to illuminating the nature of these superstructures.
For example, high quality powder X-ray diffraction patterns of nitrogen-deficient (Ca3Nx)Sn and (Ca3Nx)Pb feature barely visible reflections indicating an elpasolite-type ordering, but yield next to no information as to the extent of this ordering. The problem is compounded when looking at (Ba3Nx)Sn and (Ba3Nx)Pb, where the slight shift of barium atoms toward occupied nitrogen sites contributes much more strongly to the superstructure reflections in X-ray patterns than the occupation of the nitrogen sites itself. By contrast, the same reflections are among the strongest peaks in neutron diffraction patterns of these compounds and it is mostly the nitrogen ordering itself eliciting them.
In addition to the superstructure, (Ba3Nx)Sn and (Ba3Nx)Pb, as well as the hitherto unknown compounds (Ca3Nx)Si, (Sr3Nx)Ge and (Ba3Nx)Ge, feature distortions of the perovskite structure due to octahedral tilting. This makes the crystals undergo multiple twinning processes upon cooling down from the temperature of synthesis, which renders analysis by single crystal diffraction exceedingly difficult.

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Presenter: LINK, Lukas (Universität Stuttgart)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Structure Research

Contribution ID: **205** Type: **Poster**

Structure of Composite Materials of pNIPAM Brushes and Magnetic Nanoparticles

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Polymer chains, grafted to a substrate by one end are usually referred to as polymer brushes (PBs). They are extensively used as thin surface coatings, enabling a tuneable film thickness, as well as high chemical and mechanical stability. Further, a high versatility arises due to the various monomers that can be utilized what may cause sensitivity to external stimuli, e.g. temperature or ionic strength 1.
Since their first description and experimental realization, the range of possible shapes and applications has been growing fast and is still expanding [2]. Apart from the interesting intrinsic properties, PBs are a suitable matrix for the attachment of additional components like nanoparticles or other functional materials. In the last few years, the focus shifted more towards the interplay between PBs and other materials in order to generate specific features, like on-demand drug delivery or sensing [3].
In this work, the adsorption behaviour of citric acid capped magnetic nanoparticles (MNPs) at poly(N-isopropyl acrylamide) brushes is investigated. The MNP concentration as well as the pH value during the adsorption are varied to control the loading of the PBs with MNPs. In order to localize the MNPs at the PB, the structure of the composite material is characterized with neutron reflectometry.
1 S. Christau et al. Macromolecules, 2017, 50, pp. 7333-7343
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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

Contribution ID: **206** Type: **Poster**

Manufacturing a safer world: Residual Stress in AM determined by diffraction techniques

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Additive manufacturing (AM) technologies are experiencing a rapid growth. They promise breakthrough in engineering design (tailored parts), efficiency (environmental impact), and performance (safety). Laser Powder Bed Fusion (LPBF) is an AM method permitting the fabrication of complex structures that cannot otherwise be conventionally produced. Nevertheless, the high cooling rates associated with the process result in the formation of complex residual stress (RS) fields, which can undermine the material safety. Diffraction-based methods using penetrating neutrons and high energy X-rays at large scale facilities offer a non-destructive method to spatially resolve surface and bulk RS in complex components. These techniques also allow tracking the changes of RS following applied thermal / mechanical loads. Therefore, they represent one of the most reliable methods to assess the materials integrity in structures.
This presentation overviews some of the success stories of using large scale facilities by the BAM (the German Federal institute for Materials Research and Testing) for the determination of RS in AM metallic alloys. In particular, the study of the influence of process parameters (e.g. scanning strategies) on the RS state and the relaxation of this stress through heat treatment is presented. It is also shown how such information is used to improve the safety of AM structures. Finally, some of the challenges for diffraction-based RS analysis in AM materials are discussed.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Materials

Contribution ID: **207** Type: **Poster**

POWTEX –Angular- and Wavelength Dispersive, High-Intensity Neutron TOF Diffractometer

Wednesday, December 9, 2020 5:40 PM (20 minutes)

POWTEX is a TOF neutron powder diffractometer under construction at MLZ. Funded by Germany's Federal Ministry of Education and Research (BMBF), it is built by RWTH Aachen University and FZ Jülich, with contributions for dedicated texture sample environments from the Geo Science Centre of Göttingen University.
An instrument overview and the advances made in neutron instrumentation will be presented. Several new concepts were developed including a novel 10B detector and a double-elliptic neutron-guide system sharing focal points at the positions of pulse chopper and sample. The common focal point is an "eye of a needle"in time and space, optimizing time resolution and reducing the source background. The guide features an octagonal cross section with graded super-mirror coating, which results in Gaussian intensity and divergence distributions. The innovative jalousie detector based on solid 10B is a development for POWTEX that achieves high efficiency for a remarkably large coverage of nine steradians with almost no blind spots.
POWTEX aims for short measurement times and gives access to in situ chemical experiments, e.g., phase transitions as a function of T, p, and B0. For texture analysis, in situ deformation, annealing, simultaneous stress, etc., the large angular coverage drastically reduces the need for sample tilting/rotation. We developed new algorithms for refining angular- and wavelength-dispersive data sets (intensity as function of 2θ and λ).

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Presenter: MEINERZHAGEN, Yannick

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Neutron Methods

Contribution ID: **208** Type: **Poster**

The Fierz interference term and recent PERKEO III measurements

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron beta decay is an excellent system to test the Standard Model theory of the weak interaction and the structure of the charged weak interaction. The Fierz term is one of these parameters to study and as such is sensitive to hypothetical scalar and tensor interactions. These interactions are currently most strongly constrained by combining measurements of λ, τ and super-allowed nuclear decays.
In the past, experiments at the ILL have determined the ratio of axial-vector and vector coupling constants λ=g A /g V and the CKM matrix element V_ud in the decay of free neutrons with measurements of the β-asymmetry parameter A and of the neutron lifetime τ. The aim of the current measurement presented in this poster by PERKEO III, which was conducted until recently, is the determination of the Fierz interference term b with a precision of 5×10 -3 from the spectrum of the electrons directly.
The signature of a hypothetical non-zero Fierz term in neutron beta decay is an extra energy-dependent phase-space contribution. Major systematic effects are hence related to the detector response: calibration, temporal stability, spatial uniformity and non-linearity. With the latest measurement at ILL, we aim to obtain for the first time competitive neutron data with an existing and proven instrument, improving on the only previous result by UCNA (Los Alamos) by a factor of 20, and also establishing the necessary understanding of systematics for future measurements with PERC at the FRM II.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Nuclear/ Particle Physics

Contribution ID: **209** Type: **Poster**

The high resolution neutron backscattering spectrometer SPHERES

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The neutron backscattering spectrometer SPHERES (SPectrometer for High Energy RESolution) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It covers a dynamic range of ± 31μeV with a high resolution of about 0.66μeV and a good signal-to-noise ratio. The instrument performance has been improved over the recent years by different measures. The intensity has been more than doubled by the upgrade of the PST chopper and the focusing guide. The signal-to-noise ratio can be significantly improved by employing the new background chopper.
SPHERES enables investigations on a broad range of scientific topics from the classical applications of backscattering like hyperfine splitting or rotational tunneling to investigations on new materials like high temperature polymer electrolyte fuel cells or novel nano-composites. It is in particular sensitive to the incoherent scattering from hydrogen and allows to access dynamic processes up to a timescale of a few ns. It is hence well suited to study the dynamics in soft-matter materials like polymers or proteins, or to observe the motion of water in confined geometry. Other typical applications include relaxation in viscous liquids or diffusion processes in various systems.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **210** Type: **Poster**

Impact of ethylenediaminetetraacetate ligands on CdS nanoparticle formation mechanism

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Organic ligands are commonly employed to stabilize nanoparticle sizes, shapes and long-term colloidal stability in dispersions. For Cadmium chalcogenides, ethylenediaminetetraacetate (EDTA) seems a good candidate due to its strong chelating action towards Cd2+. Further, EDTA-capped CdS nanoparticles were proven to be stable in aqueous dispersion at room temperature over months.[1,2] Without ligands, the CdS nanoparticles nucleate via a two-step formation mechanism involving Cd13S4(SH)18 precursor particles and a diffusion-driven growth process to ca. 5 nm particles within 2.5 ms.[3] Yet, up to now no mechanistic insight into the CdS particle formation in presence of EDTA has been provided.
Here we evidence the formation of ca. 5 nm sized EDTA-capped CdS particles from CdCl2/EDTA and Na2S stock solutions with SANS and laboratory SAXS. The mixing speed and / or solvent (H2O / D2O) seem to impact the particle diameter. Contrast matching in SANS not only accesses the ligand shell, but also reveals an unexpected superstructure formation on a time scale of hours. pH-dependent studies and multinuclear and multidimensional solid-state NMR spectroscopy complement insight into the EDTA binding.[4]

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Soft Matter

Contribution ID: **211** Type: **Talk**

Cool Pressure: Implementing cryogenic temperatures at the high-pressure instrument SAPHiR

Tuesday, December 8, 2020 5:35 PM (25 minutes)

SAPHiR is a 6-6 multi-anvil instrument in the new eastern neutron guide hall of FRM II dedicated to high pressure, high temperature neutron powder diffraction and radiography, which is currently operated offline. Pressures of more than 15 GPa are available, with an internal resistance furnace providing a temperature range between room temperature and ca. 2000 ℃. However, experiments below room temperature have previously not been possible. Here, we present a new cooling system that is capable of cooling samples to ca. 120 K, thereby allowing controlled static and deformation experiments at variable P and T under cryogenic conditions to be performed. The system consists of cooling rings that enclose the base of each of the secondary anvils. The rings are flushed by liquid nitrogen, cooling the secondary anvils and the sample to 120 K in 40 min, which significantly undercuts the previous low-temperature record of multi-anvil presses by 100 K. Some applications of this new system include; static and deformation experiments of high pressure ices and clathrates suggested to exist in the interior of icy moons such as Titan; fundamental crystallography; mapping of phase diagrams; and material sciences. Neutron measurements will commence when the infrastructure is completed, but the instrument is already available for external users for offline test experiments.

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Presenter: HOWARD, Christopher (BGI)

Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **213** Type: **Talk**

Ion selectivity at the origin of block copolyelectrolyte micelle formation

Thursday, December 10, 2020 2:00 PM (15 minutes)

Novel block copolymers consisting of two anionic polyelectrolyte blocks [NaPA and NaPSS] have been synthesized. In the presence of certain amounts of divalent cations such as Calcium, Strontium and Barium, supramolecular structures are formed. The overall size and molecular weight of these structures have been obtained by combined static and dynamic light scattering (SLS & DLS). Via small-angle neutron scattering (SANS) the existence of core-shell micellar structures could be proven [1, 2]. Additional experiments using a deuterated polyacrylic acid block enabled us to elucidate the micellar composition. Core-shell structures are formed because the two charged polymer blocks possess different complexation affinities with respect to oppositely charged cations.

In a next step, solutions which are still in the single chain region of the phase diagram, but close to the phase boundary, have been prepared. Playing with temperature we succeeded in triggering micelle formation [3]. Decreasing the temperature induced micelle formation with Barium and Strontium, but not with Calcium. Surprisingly, the micellar structures were inverted in composition. Heating these solutions up to ambient temperature led to a dissolution of the micellar aggregates. Heating up even further to 65℃ led again to a formation of micelles.

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Primary authors: SCHWEINS, Ralf (Institut Laue - Langevin); PREVOST, Sylvain (Institut Laue Langevin); Dr CARL, Nico (Institut Laue - Langevin); Prof. HUBER, Klaus (Universität Paderborn)

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Session Classification: DN2020. Soft Matter

Track Classification: DN: Soft Matter

Contribution ID: **214** Type: **Talk**

Vortex Matter of Intertype Superconductors studied by Neutron Methods and Molecular Dynamics Simulations

Thursday, December 10, 2020 2:30 PM (15 minutes)

In the intermediate mixed state (IMS) in superconducting niobium, the mixed attractive/repulsive vortex interaction leads to the clustering of vortices into domains. Not fitting into the conventional type-I and type-II categories, this regime is denoted intertype superconductivity 1.

Using a combination of neutron techniques, we have studied the hierarchical properties of the IMS in bulk niobium on length scales of the vortex lattice (~100nm, SANS), the domain structure (~10mum, VSANS/USANS) and the sample size (~10mm, NGI). The results give detailed insight into the properties of the IMS focusing on the domain formation as function of temperature, magnetic field and sample quality [2,3,4].

However, the knowledge of the nanoscale vortex arrangement is still incomplete, including the domain structure and the impact of disordered vortices. In order to complement the experiments we have used molecular dynamics simulations. In a novel approach, the vortex interactions are based on an extended Ginzburg-Landau formalism 1. The focus of the simulations was on the influence of pinning and the external field on the IMS. Our combination of neutron techniques with molecular dynamics simulations pave the way to a quantitative analysis of vortex matter of intertype superconductors.

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Session Classification: DN2020: Magnetism

Track Classification: DN: Magnetism

Contribution ID: **215** Type: **Poster**

Neutron yield measurements for Be, V and Ta targets from 22-42 MeV proton beams

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The High Brilliance neutron Source (HBS) project aims to develop a scalable Compact Accelerator-driven Neutron Source (CANS) enabling neutron fluxes at the corresponding instruments comparable to medium-flux fission-based research reactors. For scalable CANS, the target material providing the largest neutron yield depends on the energy of the sub-100 MeV primary proton beam. Simulations based on the TENDL database suggest that low-Z materials, e.g. Beryllium and Vanadium, generate more neutrons at proton beam energies below 20 MeV while high-Z materials, e.g. Tantalum, generate more neutrons at proton beam energies above 20 MeV. In order to improve the reliability of the underlying databases, the neutron yield of $\mathrm{p} + \mathrm{Be}$, $\mathrm{p} + \mathrm{V}$ and $\mathrm{p} + \mathrm{Ta}$ for 22, 27, 33 and 42 MeV protons is indirectly determined by a novel method through the measurement of the 2.23 MeV gamma ray of hydrogen induced by thermal neutron capture in a polyethylene moderator. The neutron to gamma conversion rate is measured with an AmBe calibration neutron source. Corrections for escaped neutrons are applied via an MCNP simulation of the experiment. This contribution presents the experimental results and a comparison with the neutron yield obtained from simulations.

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Presenter: RIMMLER, Marius

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **216** Type: **Talk**

Destruction of long-range magnetic order in Cu_2GaBO_5 and Cu_2AlBO_5 ludwigites by an external magnetic field.

Tuesday, December 8, 2020 4:15 PM (25 minutes)

Ludwigites are oxyborate compounds with the general formula $M_2^{2+}M'^{3+}BO_5$. Their structure consists of low-dimensional zigzag walls with triangular motifs, making them an interesting playground for the realization of magnetic frustration on quasi-low-dimensional lattices. Of particular interest are copper ludwigites, in which the divalent transition-metal ion is Cu^{2+}, carrying a quantum spin 1/2, whereas the trivalent ion is nonmagnetic. Cu_2GaBO_5 and Cu_2AlBO_5 ludwigites have been careful characterized. Both compounds order antiferromagnetically with $T_N \approx 4.1$ K and 3 K, respectively. Propagation vector for Cu_2GaBO_5 is $(0.45\ 0\ -0.7)$, which was determined by diffraction measurement. We also collected μSR data as a function of temperature and weak longitudinal magnetic field. They indicate a decoupling in weak fields of about 2000 gauss, which suggests that the internal field experienced by the muon is unusually weak. On the other hand, magnetic field also induces a very fast depolarization of some small fraction of the muons, leading to a decrease in initial asymmetry, which is consistent with field-induced magnetic disorder. We also present inelastic neutron scattering measurements evidencing diffuse low-energy spin fluctuations associated with such a crossover. We suggest that these investigation help understand magnetic ordering and will be an additional step towards understanding the quantum spin system.

Primary author: KULBAKOV, Anton

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Presenter: KULBAKOV, Anton

Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

Contribution ID: **217** Type: **Talk**

Characterization of Phosphide-Based Lithium Ion Conductors by Neutron Powder Diffraction

Tuesday, December 8, 2020 3:00 PM (25 minutes)

In order to attain fast lithium conducting solid electrolytes for the development of high-energy-density all solid state batteries phosphide-based materials have recently gained much interest. With the phosphidotetrelates Li8TtP4 (Tt = Si,Ge) and Li14TtP6 (Tt = Si,Ge,Sn) several lithium conducting materials are already discovered which achieve conductivities up to 1.7mS/cm at RT.[1-4] Recently we extended this material class with the novel superionic conductor Li9AlP4 which has as an undoped material a remarkable fast ionic conductivity of ~3mS/cm at RT and a low activation energy of ~29kJ/mol.[5] Neutron powder diffraction analysis confirms the Li sub-lattice in Li9AlP4 with partial occupied and even lithium split positions. Temperature-dependent measurements reveal the phase transformation from an ordered into a disordered modification which exhibits the same structure type as found in Li14SiP6. Furthermore the crystal structures of the new compound Li8SnP4 was thoroughly analyzed by neutron powder diffraction and other methods. Maximum entropy and one-particle potential evaluations of nuclear density maps give insights into the 3D lithium ion diffusion.

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Presenter: STRANGMÜLLER, Stefan

Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **218** Type: **Poster**

PANDA - the cold neutron TAS at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The cold three axes spectrometer PANDA offers high neutron flux, high resolution in momentum (Q) and energy (E) combined with low instrumental background. The instrument allows the investigation of systems where small sample sizes are available, or samples with weak scattering cross sections. Specialized sample environment is available for experiments under extreme conditions, such as milli-Kelvin temperatures and magnetic fields up to 12 T. Furthermore, high temperatures up to 2100 K and high pressures are possible. The instrument is perfectly suited for the investigations of magnetism and superconductivity on single crystals at low energy range. Typical experiments include quantum magnetism, heavy-fermion or low-dimensional systems, frustrated and multiferroic materials, investigation of magnetic excitations, lattice dynamics and their hybridization. The actual scientific goals are often connected with discovering exotic spin states under extreme conditions and make the PANDA an excellent tool to solve the pressing questions in modern condensed matter physics.

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Presenter: SCHNEIDEWIND, Astrid

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **219** Type: **Talk**

Structure and relaxation dynamics in porous systems: A neutron scattering view

Tuesday, December 8, 2020 4:15 PM (25 minutes)

Fluids play a main role in determining the final structural and transport properties in several solvated systems like hydraulic binders1, hydrogels[2], organogels[3] and colloids in general. Thanks to their peculiar neutron-sample interaction, neutrons are the elective probe to study many hydrogen-rich systems. For this reason, neutron scattering techniques are unique in defining porous matrix topology at the nanoscale and relaxation properties in the ps-ns regime. This presentation reviews few examples were neutron scattering, even in time-resolved mode, could be of great advantage for the material intrinsic understanding and improvement.
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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **220** Type: **Talk**

(Elastic) neutron scattering on hydrogen rich samples

Tuesday, December 8, 2020 4:15 PM (25 minutes)

(Elastic) neutron scattering on hydrogen rich samples

Estimating the resolution of instruments equals predicting their capabilities. Of course, those estimates are only that good as the assumed simplifications are justified. One of the most significant assumption for SANS or NR is, that they are solely elastic. In this context, the interaction of neutrons with hydrogen rich samples is of particular interest, especially due to numerous neutron scattering experiments investigating soft condensed matter. Without doubt, the contribution of elastic scattered neutrons is by far dominating. However, resolving scattering features, which require high signal to noise ratio or q-resolution, are limited by in- and or quasi-elastic scattered neutrons. The same circumstances might also restrict the significance of the outcome of commonly used contrast variation experiments, originated by the strong incoherent scattering length and fast dynamics of 1H compared to deuterium. Here we will present SANS and NR experiments showing inelastic / quasi-elastic scattering, partially compare them to spectroscopic investigations in the same scattering geometry and elaborate their impact on data quality.

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Presenter: SOLTWEDEL, Olaf

Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **221** Type: **Poster**

Rotational and long range diffusion in a lithium amide–lithium borohydride mixture

Wednesday, December 9, 2020 5:40 PM (20 minutes)

On-board hydrogen storage is still a challenge for fuel cell vehicles and other mobile applications. Complex hydrides, which contain ions such as BH4- and NH2-, have a high hydrogen capacity in combination with a low weight of the storage material. For example, Li4BH4(NH2)3 contains 11.1 wt.% hydrogen and desorbs more than 10 wt% at 573-673 K. In previous studies the high desorption temperature was reduced with additives. To understand the chemical behaviour and atomic motions of Li4BH4(NH2)3, we present an in situ phase analysis and quasielastic neutron scattering (QENS) during heating.
In situ X-ray diffraction was measured up to 573 K at P02 (DESY) and QENS was taken at TOFTOF (MLZ) in the temperature range 300-514 K. Li4BH4(NH2)3 melts at 494 K and during heating crystallization of a second phase was detected and identified as LiNH2, which remained a crystalline residue in the melted material. From the quasielastic signal rotational and long range motions were analysed and assigned to BH4- and NH2- of Li4BH4(NH2)3 and of the crystallized LiNH2 phase.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **222** Type: **Poster**

A buffer-gas trap for the NEPOMUC high-intensity low-energy positron beam

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The APEX collaboration aims to produce a neutral pair plasma, comprised of equal quantities of electrons and positrons, confined by the magnetic field of a levitated dipole. More than 10^{10} positrons are needed to achieve a short-Debye-length plasma with a volume of 10 litres and a temperature of $\sim$ 1~eV, which necessitates new advances in positron accumulation. Buffer-gas positron traps have dramatically extended the scope for atomic and non-neutral plasma physics experiments involving antimatter. In these devices, a continuous beam of positrons enters a Penning-Malmberg trap, wherein inelastic collisions with low-density molecular gases promote the efficient capture of the antiparticles. We present our plans for the installation of a buffer-gas trap at the NEPOMUC neutron-induced positron source in Munich. Beyond the pair plasma experiments, an intense trap-based positron beam will also facilitate new applications, for example, the background-free measurement of positron-annihilation-induced Auger-electron spectra.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **224** Type: **Talk**

Instrumentation at a compact accelerator-based neutron source

Thursday, December 10, 2020 3:45 PM (15 minutes)

Compact accelerator-based neutron sources (CANS) produce neutrons by low energy nuclear reactions well below the spallation threshold making them a cost-efficient and effective alternative to spallation and reactor based neutron sources. Such low energy (p, n)-reactions produce less and lower energy byproducts thus reducing significantly the radiation level. This allows the construction of a very compact target / moderator / reflector (TMR) unit with a thermal and cryogenic moderator placed close to the target providing a high phase space density or in other words a high brilliance neutron source. The compact design and the low radiation level allow the placement of optical elements close to the moderator surface, e.g. neutron guides or choppers, thus allowing the extraction of large phase space volumes with a large brilliance transfer to the sample. The instrumentation at a high power CANS with a proton beam power in the range of 100 kW, which we investigate in the framework of the HBS project, can be competitive to instruments at spallation sources with comparable beam power and current operated research reactors.

At the DN2020, I will present the potential a high power CANS offers for the design of different instruments e.g. reflectometer, SANS or spectrometers.

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Session Classification: DN2020: Instrumentation

Track Classification: DN: Instrumentation

Contribution ID: **225** Type: **Poster**

Multiple Length Scales Hydration in Polymer Membranes for Fuel Cells

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The polymeric materials used in fuel cells applications either as proton (PEMFC) or anion (AEMFC) exchange membranes are characterized by a nanoscale phase separation into hydrophilic domains and hydrophobic crystalline regions, which enables a high conductivity and provides a good chemical and mechanical stability of the membrane. Owing to its high proton conductivity and chemical stability, Nafion was established as benchmark for PEMFC applications. However, due to its high cost and limitations in operating conditions, there is an intense search for low-cost alternative materials with similar conductive and chemo-mechanical properties. On the other hand, the high proton conductivity in PEMFC is achieved in acidic environment that requires the consumption of acidic-resistant precious metal catalysts and impedes a wide-scale commercialization. As alternative technology, the AEMFC use inexpensive, non-noble metal catalysts. However, the AEM conductivity and long-term durability is still lower compared to the PEM, therefore the interest in finding new high-performance materials. The conductivity in polymer electrolyte membranes depends on the water behavior inside the polymer network across the full range of length scales in the membrane. As we will present here, small-angle neutron scattering with contrast variation used at MLZ is a powerful technique for unraveling the hierarchical morphology and understanding the structure–property relationships in such polymeric membranes.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **226** Type: **Talk**

Interdependent scaling of long-range oxygen and magnetic ordering in non-stoichiometric Nd2NiO4.10

Tuesday, December 8, 2020 1:40 PM (25 minutes)

Hole doping in Nd2NiO4.00 can be either achieved by substituting the trivalent Nd atoms by bivalent alkaline earth metals or by oxygen doping, yielding Nd2NiO4+δ. While the alkaline earth metal atoms are statistically distributed on the A-cation sites, the extra oxygen atoms in interstitial lattice remain mobile down to ambient temperature and allow complex ordering scenarios depending on δ and T. Thereby the oxygen ordering, usually setting in far above room temperature, adds an additional degree of freedom on top of charge, spin and orbital ordering, which appear at much lower temperatures. In this study, we investigated the interplay between oxygen and spin ordering for a low oxygen doping concentration i.e. Nd2NiO4.10. The presence of a complex 3D modulated structure related to oxygen ordering already at ambient was evidenced by single crystal neutron diffraction, the modulation vectors being ±2/13a±*3/13b*, ±3/13a±*2/13b*and ±1/5a±*1/2c* with satellites up to fourth order. The coexistence of oxygen and magnetic ordering below TN ⊠ 48 K was evidenced, with magnetic satellite reflections adapting the same modulation vectors as found for the oxygen ordering, evidencing a unique coexistence of 3D modulated ordering for spin and oxygen ordering in Nd2NiO4.10. Temperature dependent measurements of magnetic intensities suggest two magnetic phase transitions below 48 K and 20 K, indicating two distinct onsets of magnetic ordering for the Ni and Nd sublattice, respectively.

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Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **227** Type: **Poster**

Replacing MultiView and LabView with NICOS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

MGML (Materials Growth & Measurement Laboratory) in Prague is an open research infrastructure providing access to the instrument suite dedicated to measurements of a rich spectrum of physical properties of materials in a wide range of temperatures, magnetic and electrical fields, and hydrostatic uniaxial pressures. Together there are 18 furnaces, 3 diffractometers, 5 room temperature instruments and 8 cryostats.
NICOS software 1 is used on every instrument as an experimental logbook, providing user authentication against user office system and uploading measured data after experiment to central file storage. All cryostats can be controlled with NICOS: Cryogenics 20T magnet, Leiden Cryogenics 9T magnet with dilution insert and Oxford Instruments Triton cryofree dilution refrigerator with 4T vector magnet. All Quantum Design instruments (3x PPMS, 2x MPMS) can be also controlled with NICOS via SECoP [2].
We will present a way how to use NICOS for resistivity measurement (Keithley K6221/K6220 + K2182A, DC using Delta method, up to few GΩ or Lock-In Amplifier SR830(+K6221), SR865, up to 4MHz and also Keithley K6517B, DC, up to and beyond TΩ). Special setup also exists for measurement of thermal conductivity and Seebeck coefficients.
Our users are happy to use instrument friendly software and in addition they are used to NICOS when they will come to neutron facility for the first time.

1 https://nicos-controls.org/
[2] https://github.com/SampleEnvironment/SECoP

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **228** Type: **Poster**

Current Status of PERC

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The PERC (Proton and Electron Radiation Channel) facility is currently under construction at the MEPHISTO beamline of the FRM II, Garching. 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. It hosts an 8 m long decay region in a uniform field. An additional high-field region selects the phase space of electrons and protons, which can reach the downstream detector and systematic uncertainties.
The downstream main detector and the two upstream backscattering detectors, will initially be scintillation detectors with (silicon) photomultiplier readout. In a later upgrade, the downstream detector will be replaced by a pixelated silicon detector.
Delivery of the magnet system is scheduled before the end of this year. We present details on PERC's current status.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **229** Type: **Talk**

Multiple phase transitions in HoFeO3 determined by single crystal neutron diffraction in applied magnetic field

Tuesday, December 8, 2020 5:10 PM (25 minutes)

The scientific interest the rare-earth orthoferrites RFeO3, known over decades, relive significantly in the last years due to the discovery of multiferroicity or magnetocaloric effect in this family of compounds. Their remarkable magnetic properties result from complex interactions between the 3d electrons of the transition metal and the 4f electrons on the rare-earth. HoFeO3 is one of the most interesting representatives of RFeO3 family with strong magnetic interactions and a number of reorientation transitions. It has centrosymmetric space group Pnma, and Fe sub-lattice orders AFM at TN = 640 K. At zero field the Fe sub-lattice starts to polarize Ho magnetic order at about 60 K. The magnetic structure has several different phases described by magnetic irreducible representations: Γ4 = Γ_(4+)Fe ⊕ Γ_(4-)Ho, Γ1 = Γ_(1+)Fe ⊕ Γ_(1-)Ho, Γ2 = Γ_(2+)Fe ⊕ Γ_(2-)Ho. Our results, obtained under application of magnetic field along crystal axis c, show, that at low field the transition from phase Γ4 to Γ1, where Fe3+ moments rotates from c to a direction take place not directly in the ac plane, but over an intermediate phase with moments along b axis braking the centrosymmetry. The magnetic phase Γ1 disappears completely in magnetic fields above 2.5 T. Further intermediate magnetic phase in the temperature range of 8-25 K is suppressed by magnetic fields above 1 T. This behavior of HoFeO3 in weak magnetic fields makes it a good candidate for research on magnetocaloric effect.

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Presenter: OVSIANIKOV, Aleksandr

Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **230** Type: **Talk**

Neutron optics for PERC

Tuesday, December 8, 2020 1:40 PM (25 minutes)

The PERC experiment is currently under construction at the new beam port MEPHISTO at the FRM II. It aims to measure correlation parameters in neutron beta decay with an accuracy improved by one order of magnitude to a level of 10^{-4}.
Inside the PERC instrument, an 8 m long neutron guide contains the decay volume in a magnetic field of 1.5 T and is fed by a highly polarized cold neutron beam. In order to ensure a depolarization of the neutron beam on the level of 10^{-4} per bounce, completely non-magnetic coatings preferably made of diamagnetic materials are required. We present measurements of new supermirrors made from copper and titanium layers with excellent reflectivity. Despite the well-known high mobility of copper, which leads to degradation of the reflectivity caused by interdiffusion, our supermirrors are highly resistant to baking-out needed to fulfill the requirement of low residual gas pressure.
We also present results on solid-state neutron polarizers made with Iron/Silicon coatings. These polarizers are based on neutron transmission through the polarizer substrate. This opens the opportunity to choose a substrate material with higher neutron optical potential than the potential of the Fe for neutrons with spin antiparallel to the magnetic holding field, which eliminates total reflection of the unwanted spin component even in the low q-region. Main advantages are high degree of polarization over wide angular range as well as a very compact construction.

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Presenter: HOLLERING, Alexander

Session Classification: MLZ Users 2020 - Nuclear, Particle, and Astrophysics

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **231** Type: **Poster**

Bambus: introducing a new inelastic neutron multianalyser for Panda at MLZ

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Cold-neutron triple-axis spectrometers (TAS) are focused on the investigation of low-energy excitations within condensed matter physics, covering a broad selection of topics from superconductivity to magnetism. The original design of this type of spectrometer measures an individual point in a large (Q, E) space for each instrument setting. In order to increase the useful signal on TAS, recently a new form of detector design was envisioned which allows for the measuring of multiple points in (Q, E) space simultaneously. Concordantly, the multianalyser BAMBUS is being developed and constructed at the spectrometer PANDA at MLZ, in cooperation with TU Dresden and with financial support from the BMBF. The concept is to collect data at multiple points along curved paths in reciprocal space at multiple energy transfers by using multiple analysers with fixed positions, with the aim of building up a broad map in a comparatively short period of time. The aim is to use this as a complementary option to the traditional setup within single experiments, and so a fast switching time between the two options is envisioned. The aim is to improve both the versatility and data collection of the spectrometer PANDA.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **232** Type: **Talk**

The singlet-triplet gap structure of the noncentrosymmetric superconductor Ru7B3

Tuesday, December 8, 2020 5:35 PM (25 minutes)

Noncentrosymmetric (NCS) materials present an interesting environment for superconductivity, as parity is no longer a conserved quantity, leading to the possibility of superconducting systems with a superposition of s-wave and p-wave states. Such systems are predicted to have unusual properties, such as large Pauli limiting fields and 'helical'vortex states. The dependence of the superfluid density on temperature is determined by the gap function, and therefore measuring this is one method to probe the presence of mixed superconducting states predicted for NCS superconductors. We have used small-angle neutron scattering from the vortex lattice on the SANS-I instrument at MLZ to investigate this in the NCS superconductor Ru7B3, a system which has already demonstrated highly unusual vortex behaviour where the structure of the vortex lattice shows a dependence on the field-history of the system in a manner not explicable by any established theory or through a mechanism such as vortex pinning. Our measurement of the temperature dependence of the superfluid density indicates that Ru7B3 is not a pure s-wave superconductor, and in-fact demonstrates the predicted s-wave and p-wave admixture from a recent theoretical model which has shown success in describing other NCS superconductors.

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Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

Contribution ID: **233** Type: **Poster**

An insight into the local structure and dynamics of A2Zr2O7

Wednesday, December 9, 2020 5:40 PM (20 minutes)

$A_2Zr_2O_7$ oxides have been studied partially because of their possible use in the storage of nuclear waste (1) or as a photochemical catalyst materials (2). The overall $A_2Zr_2O_7$ structure is cubic (of pyrochlore type for light rare earth, defect-fluorite type for heavy rare earth ones). The pyrochlore zirconates are thoroughly investigated quantum spin ice candidates, whereas heavy rare earth zirconates remains understudies - high temperature and specially application focused studies have been reported. The material behaviour important for the upper mentioned applications strongly depends on the actual crystal structure. We present the results on (i) bulk properties of an $Er_2Zr_2O_7$ single crystal investigated by means of specific heat, magnetization and AC susceptibility, all revealing a glass-like anomaly at 2 K. (ii) the microscopic properties investigated by total neutron scattering. The pair distribution function shows the deviation from the long-range defect-fluorite structure. (iii) the muon spin rotation spectroscopy performed to reveal the nature of anticipated spin glass state at low temperature showing persisting strong spin dynamics not consistent with classical spin-glass systems. The results are discussed in a wider context of frustrated and magnetically diluted systems.

(1) K. E. Sickafus, L. Minervini, R. W. Grimes, J. A. Valdez et al., Science 289, 748 (2004).
(2) T. Omata and S. Otsuka-Yao-Matsuo, J. Electrochem. Soc. 148, E475 (2001).

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Magnetism

Contribution ID: **234** Type: **Poster**

Magnetic scattering of polarized neutrons on structures of reduced graphene oxide embedded in the polystyrene matrix

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The development of composite materials based on graphene, included in polymer matrices of different nature, and the study of the relationship between their structure and properties using complementary methods of research are due to several reasons. First is the search for new magnetic materials promising in spin electronics. Second, there is interest in physical processes in highly defective nanostructured carbon materials, in which, according to literature data, magnetic and superconducting effects may occur. In this study, for the first time, using the method of small-angle polarized neutron scattering (SAPNS), an assessment of the scale of arising spin correlations in reduced graphene oxide (RGO), which was preliminarily surface-modified with 3-(trimetoxysilylpropyl)methacrylate (TMSPM) and copolymerized with styrene, was made. Two-dimensional RGO structures functionalized by vinyl groups and embedded in the polystyrene matrix were measured using the SAPNS method (FRM-2, KWS-1, Garching). The SAPNS experiments showed the presence of magnetic-nuclear interference both in the modified TMSPM carbon filler and in the polystyrene/RGO composite, which indicates the presence of magnetized areas of 1000 Å scale and magnetic scattering with amplitude B≠0 in the systems under study.
The work was supported by RFBR grant № 20-02-00918 A.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **235** Type: **Talk**

Chlorine determination in archaeological iron artefacts by PGAA

Tuesday, December 8, 2020 2:05 PM (25 minutes)

Archaeological iron finds often undergo a secondary destructive corrosion process after excavation. Since chlorine is supposed to play a major role in this process, it is important to have a method for determining the chlorine content of such objects non-destructively, both for assessing the danger of corrosion and to verify the efficiency of methods trying to remove the chlorine. Neutron activation analysis (NAA), and prompt gamma activation analysis (PGAA) in particular, is the method of choice for the Cl determination in archaeological iron artefacts. By PGAA, sizeable pieces can be studied in a non-destructive manner with a detection limit of about 10 ppm. Since hardly any long-lived radioactivity is produced, the objects can be returned to museum collections within weeks after the analysis. We will report on studies of a large number of mainly Celtic iron artefacts from Bavaria that were excavated in the past 150 years and are in various states of preservation. Space-resolved Cl determination helps to understand details of the corrosion process. The efficiency of the removal of Cl from ancient objects by heating and leaching processes has been studied. The Cl removal from artificially corroded iron specimens prepared in the laboratory was studied in order to obtain a better understanding of the chemical bonding of the Cl that can be removed by the different methods.

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Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **236** Type: **Poster**

Liquid dynamics of phase-change materials

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Phase-change materials can be rapidly and reversibly switched between the amorphous and crystalline states in a few nanoseconds. They have been successfully employed for non-volatile phase-change memory applications. However, the dynamics of atomic rearrangement processes and their temperature dependence, which govern their ultrafast switching, are not fully understood. Here, using quasi-elastic neutron scattering, we investigate the liquid-state dynamics of a phase-change material Ge15Sb85. With time-of-flight spectroscopy, we measured dynamic structure factors as a function of temperature. The characteristic relaxation times can be extracted at the structure factor maximum, and the mean self-diffusivity of atoms are determined at the low-q range. The relaxation times of Ge15Sb85 are smallest compared with the other phase-change materials such as Ge2Sb2Te5. The mean self-diffusivity of Ge15Sb85 is higher than Te-rich alloys. This indicates that Sb-rich alloys have faster liquid dynamics than Te-rich alloys. This may partially explain the difference in their crystal growth velocities. We show that the relaxation times extracted from neutron scattering are proportional to macroscopic viscosities. A breakdown of Stokes-Einstein relation is observed in all investigated compositions, which can be attributed to the formation of locally favored structures. The latter is likely associated with the liquid-liquid transitions revealed by a recent femtosecond X-ray diffraction study.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **237** Type: **Poster**

Enhancing the High-Temperature Strength of a Co-Base Superalloy by Optimizing the y/y' Microstructure

Wednesday, December 9, 2020 5:40 PM (20 minutes)

The newly developed polycrystalline Co-base superalloy CoWAlloy2 provides a high potential for application as wrought alloy due to the large gap between solidus and y' solvus temperature along with a high y' volume fraction. The scope of this study was to maximize the high-temperature strength and to optimize the y/y' microstructure by adjusting the multi-step heat treatments.
The microstructure and mechanical properties were investigated by scanning electron microscopy (SEM), transmission electron microscopy (TEM), compression and hardness tests. In-situ high temperature small angle neutron scattering (SANS) helped to understand the microstructural evolution during different applied heat treatments. The size of the y' precipitates increases with increasing annealing time and temperature of the first annealing step. As a result, the hardness of the alloy increases until a maximum after 4 h annealing is reached. The reason is an optimum y' precipitate size in the range of about 30-40 nm, which can be explained by the model for shearing of the y' precipitates by weakly and strongly coupled dislocations. A second annealing step leads to a further increase of yield strength due to an exceptionally high y' volume fraction of about 70%. The room temperature yield strength of the optimized condition is 140 MPa higher compared to the other heat-treated condition.

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Presenter: HAUSMANN, Daniel

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science

Contribution ID: **238** Type: **Poster**

Pharmaceutical Drug Carriers organized in Nano-Domains –Study and Design upon Neutron Scattering with contrast variation, SAXS and DLS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Specific target Nanoparticles for therapy of cancer and other diseases were assembled from lipids, polymers, and pharmaceutical drugs or mRNA. For cell targeting proteins were bound to the surface (corona). The structure in solution is analyzed by dynamic light scattering DLS combined with neutron small angle scattering SANS, SAXS, metal specific X-ray scattering ASAXS. Material sub-domains in the nanoscaled drug carriers (100 nm, polymer complexes, liposomes) were localized by contrast variation.
The nanoparticles, e.g. biodegradable polymer (PLGA, Carbohydrates), intestinal lipid-bile nanoparticles, lipid particles, proteins and optional bio-target domain are ampiphilic. Thus the internal particle structure forms sub-domains of different material and scattering power, enabling a localization by contrast. For several medical cases we construct and study pharma nanoparticles for parenteral and oral applications, which contain soluble or hydrophobic drugs, or nucleic acid drugs, e.g. mRNA. Cell or tumor recognition and uptake of the drug carriers can obtained by a surface protein, ligand head.
mRNA nano-complexes for immune-vaccination and cancer therapy work by cellular synthesis of the corresponding protein (not the antigen, but the genetic information for it is supplied). Oral nano-drug application is tested with a simulator device of the gastro-intestinal tract with SANS-DLS observation of drug nanoparticles and intermediates.

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Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Life Science/ Biology

Contribution ID: **239** Type: **Talk**

Nano-Structure Development of Oral Pharmaceutical Formulations in Simulated Intestine –D-contrast SANS and DLS

Tuesday, December 8, 2020 3:25 PM (25 minutes)

Pharmaceutical drug formulations for oral delivery depict after patient intake a stepwise structure development of disintegration to micro-particles, dissolution of drug nano-complexes, interaction with bile and lipids and uptake by the intestinal membrane proteins (receptors). The processes are critical for therapy and applicability of drug and formulation, especially with hydrophobic or badly soluble drugs.
The processing of oral drug formulations was studied by neutron small angle scattering SANS with D-contrast variation, combined with DLS, with a simulator device of the human gastro-intestinal tract with SANS+DLS observation of drug nanoparticles and intermediates. A set of drugs, where oral delivery is a challenge, was investigated, e.g.: Fenofibrate, Amphotericin B, Danazol, Griseofulvin, Carbamazepine, Curcumin in combination with lipids and detergents. The biocompatibility was estimated with cell cultures. The drugs were embeded in nanoparticles and liposomes of 50-100 nm size and resolved stepwise in artificial intestinal fluid and bile. The resolution and formation of intermediated nanoparticles and excipient-drug complexes was analyzed with time resolved SANS and DLS. Substructures (domains) were localized by solvent deuterium contrast variation. The results are part of the development of novel formulations of difficult drugs upon structure investigation by SANS plus DLS in a feedback process.

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Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **241** Type: **Poster**

Nano-Structure Development of Oral Pharmaceutical Formulations in Simulated Intestine –D-contrast SANS and DLS

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Pharmaceutical drug formulations for oral delivery depict after patient intake a stepwise structure development of disintegration to micro-particles, dissolution of drug nano-complexes, interaction with bile and lipids and uptake by the intestinal membrane proteins (receptors). The processes are critical for therapy and applicability of drug and formulation, especially with hydrophobic or badly soluble drugs.
The processing of oral drug formulations was studied by neutron small angle scattering SANS with D-contrast variation, combined with DLS, with a simulator device of the human gastro-intestinal tract with SANS+DLS observation of drug nanoparticles and intermediates. A set of drugs, where oral delivery is a challenge, was investigated, e.g.: Fenofibrate, Amphotericin B, Danazol, Griseofulvin, Carbamazepine, Curcumin in combination with lipids and detergents. The biocompatibility was estimated with cell cultures. The drugs were embeded in nanoparticles and liposomes of 50-100 nm size and resolved stepwise in artificial intestinal fluid and bile. The resolution and formation of intermediate nanoparticles and excipient-drug complexes was analyzed with time resolved SANS and DLS. Substructures (domains) were localized by solvent deuterium contrast variation. The results are part of the development of novel formulations of difficult drugs upon structure investigation by SANS plus DLS in a feedback process.

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Presenter: NAWROTH, Thomas (Gutenberg-University, Pharmaceutical Technology, Staudingerweg 5)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Soft Matter

Contribution ID: **242** Type: **Poster**

MIEZETOP for the cold triple axis spectrometer (TAS) MIRA

Wednesday, December 9, 2020 5:40 PM (20 minutes)

Neutron Spin Echo is a techniques to obtain high resolution which uses the spin to record information. It is used to observe slow phenomena, which are correlated to relaxation processes, e.g. correlations between atomic positions or spin orientations. Here these phenomena manifest itself in an inelastic broadening of the structure factor S(Q) revealing time domains of inelastic processes that are magnitudes higher than classical neutron spectrometers. One way of realization is MIEZE (Modulation of IntEnsity with Zero Effort) where the energy transfer displays in a contrast change of the oscillating signal. We implement this technique into our triple axis instrument to obtain high resolution in a broad Q-range.

Primary author: GABOLD, Henrik

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Presenter: GABOLD, Henrik

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: DN: Instrumentation

Contribution ID: **243** Type: **Talk**

Investigation of orthorhombic and tetragonal phases of Cs2CuCl4-xBrx mixed system

Tuesday, December 8, 2020 3:50 PM (25 minutes)

The Cs2CuCl4-xBrx mixed system exists in orthorhombic and tetragonal polymorphs and is an example of the low-dimensional quantum spin systems. The different Cu2+ environments and their influence on the magnetic properties are important to understand the change of magnetic behaviour by applying magnetic field. The orthorhombic mixed system was studied by neutron single crystal diffraction with and without magnetic field. It shows a rich magnetic phase diagram consisting of four regimes depending on the Br concentration and is characterised by different exchange coupling mechanisms. Inelastic neutron scattering experiments on MIRA for the compound from regime III (2 < x < 3.2) with x=2.2 show dynamical correlations at a temperature around 50 mK giving evidence for a spin liquid phase 1.

I4/mmm has been used to describe the tetragonal polymorphs. The magnetic behaviour of such tetragonal compounds can be described as quasi-2D antiferromagnets with a transition temperature TN between 9K and 11K, depending on the Br content [2]. New single-crystal neutron diffraction experiments on RESI indicate a very small orthorhombic distortion at low temperature. The structure solution shows a subgroup relationship for the investigated composition of this mixed system.

1 N. van Well et al., Ann. Phys. (Berlin), 2000147, (2020),
[2] N. van Well et al., Cryst. Growth Des., 19, 11, 6627-6635 (2019)

Primary author: Prof. VAN WELL, Natalija (Department of Earth and Environmental Sciences, Crystallography Section, Ludwig-Maximilians-University Munich)

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Session Classification: MLZ Users 2020 - Structure Research

Track Classification: UM: Structure Research

Contribution ID: **244** Type: **Invited talk**

Inorganic nanoparticles challenging lamellar and non-lamellar lipid membranes: the role of curvature in nano-bio interactions

Tuesday, December 8, 2020 3:00 PM (25 minutes)

The interaction of engineered nanomaterials with living systems is mediated by biological barriers, determining their biological fate and cytotoxicity. Understanding the interaction of nanoparticles (NPs) with biological interfaces is the key to fill the gap between NPs development and end-use application. Lipid-based synthetic membranes can be used to mimic natural interfaces under simplified conditions, in order to identify key determinants in nano-bio interactions. While most of investigations so far focused on lamellar models, far less attention is given to curved-bilayer structures, ubiquitous in cells under certain conditions. Here, we address the interaction of inorganic NPs with biomimetic bilayers of lamellar and non-lamellar nature, i.e. flat membranes to cubic architectures encountered in diseased cells. With a library of gold NPs, we explore the effect of NPs shape and surface coating as a function of membrane curvature. Through an ensemble of structural techniques (SAXS, GISANS and Neutron Reflectivity), we found that highly curved membranes are associated with an enhanced structural stability towards NPs. Moreover, Confocal Laser Scanning Microscopy analysis highlights that cubic and lamellar phases interact with NPs according to two distinct mechanisms. These results are the first attempt to systematically study the role of membrane curvature in the interaction with NPs, disclosing new perspectives on the understanding and application of Nano-bio Interfaces.

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Presenter: Ms CASELLI, Lucrezia (University of Florence)

Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **245** Type: **Talk**

The Robot Positioning System at the Materials Science Diffractometer STRESS-SPEC

Tuesday, December 8, 2020 3:25 PM (25 minutes)

The diffractometer STRESS-SPEC is optimised for fast strain mapping and pole figure measurements. Our group was the first to pioneer the usage of industrial robots for sample handling at neutron diffractometers. However, the current robot is limited in its use due to insufficient absolute positioning accuracy of up to ± 0.5 mm. 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 mm^3 –is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. Therefore, the original robot setup at the neutron diffractometer STRESS-SPEC is currently being upgraded to a high accuracy positioning/metrology system. We will present the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 µm or better during strain measurements the sample position will be tracked by an optical metrology system and it is going to be actively corrected. The additional use of radial collimators creates more space in the sample environment and enhance the residual stress analysis capabilities for large complex parts. Finally, a newly designed laser furnace can be mounted at the robot flange to conduct texture measurements at elevated temperatures of up to 1300 ℃. A brief overview of the STRESS-SPEC instrument and its capabilities as well as first commissioning experiments using the new setup will be given.

Primary authors: Prof. BROKMEIER, Heinz-Günter (Institute of Materials Science and Engineering -Department TEXMAT-TU Clauthal); WANG, Lijiu; LANDESBERGER, Martin (TUM); HOFMANN, Michael; Mr KEDILIOGLU, Oguz (Friedrich-Alexander-Universität Erlangen-Nürnberg); GAN, Weimin (Helmholtz-Zentrum Geesthacht)

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Session Classification: MLZ Users 2020 - Neutron Methods

Track Classification: UM: Neutron Methods

Contribution ID: **246** Type: **Invited talk**

Frequency-based decay electron spectroscopy

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Precision measurements of $\beta-$decay spectra can provide exquisitely sensitive tests of various predictions and underlying symmetry assumptions of the Standard Model (SM) of Particle Physics. Possible symmetry violations can alter the shape of β-decay spectra in characteristic ways. Beyond SM physics e.g. causes the finite masses of neutrinos that alter the $\beta-$decay spectrum of tritium in a predictable but still undetectable way. In a first step to design an experiment with a sensitivity of $40\,\mathrm{meV/c^2}$ to the neutrino mass scale the Project 8 collaboration has recently demonstrated a novel, frequency-based electron spectroscopy technique. Cyclotron Radiation Emission Spectroscopy (CRES) determines the electron's kinetic energy from the feeble cyclotron radiation emitted by an electron spiralling in a magnetic trap. I will present the basics of CRES and results obtained with mono-energetic conversion electrons from $^{83\mathrm{m}}\mathrm{Kr}$ as well as preliminary results from measurements using molecular tritium. I will discuss the prospect of CRES in the context of precision $\beta-$decay experiments of the next generation, in particular with a focus on the neutron decay spectrum.
This work has been supported by the Cluster of Excellence "PRISMA+" (EXC 2118/1) funded by the German Research Foundation (DFG) within the German Excellence Strategy (Project ID 39083149), the US DOe and NSF and by internal investments at all collaborating institutions.

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Session Classification: MLZ Users 2020 - Nuclear, Particle, and Astrophysics

Track Classification: UM: Nuclear, Particle, and Astrophysics

Contribution ID: **247** Type: **Plenary talk**

A study of vacancy-type defects in wide-gap semiconductors by means of positron annihilation spectroscopy

Wednesday, December 9, 2020 10:15 AM (45 minutes)

Positron annihilation is a non-destructive tool for investigating vacancies in materials. A positron annihilates with an electron and emits gamma rays in solids. Their energy distribution is broadened by the momentum component of the annihilating electrons. A positron could be trapped by a vacancy because of Coulomb repulsion from ion cores. Because the momentum distribution of the electrons in the defects differs from that of electrons in the bulk, the defects can be detected by measuring the energy distribution of the annihilation radiation. The electron density in vacancies is lower than that in the bulk, which increases the lifetime of positrons. Thus, the measurement of positron lifetimes is also a useful method to detect vacancies.
Using monoenergetic positron beams constructed at University of Tsukuba and TUM FRMII (NEPOMUC), we have characterized vacancies in Mg implanted GaN. Depth distributions of the defects, their annealing behaviors, and interactions with impurities were studied to achieve p-type GaN using ion implantation. The carrier trapping phenomena by vacancies were also studied. A study of native defects in AlN and their introduction mechanisms during the growth will be also presented in the talk.
This work was supported by the MEXT "Program for research and development of next-generation semiconductor to realize energy-saving society", and a part of this work was also supported by JSPS KAKENHI (Grant No. 16H06415).

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Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **248** Type: **Plenary talk**

Novel luminescence materials

Thursday, December 10, 2020 11:00 AM (30 minutes)

While the cation chemistry in many materials has been extensively studied, in the field of mixed anion compounds a lot remains to be discovered yet. Especially mixed-anionic hydrides are receiving a lot of attention at the moment, because the partial substitution can significantly change the physical and chemical properties 1. Due to the low scattering power of hydride, the combined use of neutron and X-ray diffraction is essential for a complete structural characterization.
Beside the use of these tools, also the use of local probes can be helpful. For instance, rare earth metal ions showing 5d-4f transitions can show very sensitive differences in the polarizabilities in the local environment. Recently, a number of new mixed-anionic hydrides and complex hydrides has been discovered. Here, mixed hydride halides and borohydrides are studied. Furthermore, the first representative of a novel class of materials, the borate hydride Sr5(BO3)3H:Eu2+ is presented. The successful incorporation of hydride in the later compound was shown using a number of independent methods, including neutron powder diffraction, 1H solid state MAS NMR, vibrational spectroscopy and quantum chemical calculations.

Beamtime at the SPODI, Research Neutron Source Heinz Maier-Leibnitz (FRM II) and the D2b, Institute Laue-Langevin is gratefully acknowledged.

1 Y. Kobayashi, T. Yoshihiro, H. Kageyama, Ann. Rev. Mater. Res. 2018, 48, 11.1.

Primary author: KUNKEL, Nathalie

Presenter: KUNKEL, Nathalie

Session Classification: DN2020: Plenary talks

Track Classification: DN: Plenary talks

Contribution ID: **249** Type: **Plenary talk**

Structural disorder in photovoltaic absorber materials: insights by neutron diffraction

Wednesday, December 9, 2020 9:30 AM (45 minutes)

Photovoltaics, the direct conversion from sunlight into electricity, has developed into a mature technology during recent past.
Quaternary chalcogenide semiconductors have received increasing attention as absorber material in thin film solar cells, because their constituents are abundant and non toxic. Best performing devices are obtained with off-stoichiometric kesterite-type $Cu_2ZnSn(S,Se)_4$. The strong stoichiometry deviation causes structural disorder which influences the optoelectronic properties of the semiconductor crucial.
Ternary nitrides ($ZnSnN_2$, $ZnGeN_2$) have attracted attention as potential earth-abundant alternatives to III-V absorber materials. $ZnGeN_2$ is reported to crystallise in the β-$NaFeO_2$-type structure, in which Zn^{2+} and Ge^{4+} cations are ordered. A variable degree of cation disorder was reported[1], up to full disorder (wurtzite structure). The situation becomes even more complex when taking oxygen into account: the effect of oxygen on the cation disorder from exclusive cation disorder has to be disentangled carefully.
In order to study the structural disorder in quaternary chalcogenides and ternary nitrides we applied neutron powder diffraction to differentiate the isoelectronic cations Zn^{2+}, Cu^{+} and Ge^{4+} as well as nitrogen and oxygen, deriving correlations between cation disorder, off-stoichiometry and band gap energy.
1 C. L. Melamed et al, J. Mater. Chem. C, 2020, 8, 8736

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Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **250** Type: **Plenary talk**

Quantum vs. structural disorder in triangular antiferromagnets

Thursday, December 10, 2020 11:30 AM (30 minutes)

Quantum disordered states in frustrated magnets are model cases of quantum entanglement and potential hosts for unconventional, fractionalized excitations. The formation of these states is typically associated with competing exchange couplings, although structural disorder can lead to a somewhat similar phenomenology, including the absence of long-range magnetic order and the presence of excitation continua.

In this talk, I will discuss the interplay of quantum and structural disorder in Yb-based triangular antiferromagnets that were recently proposed as spin-liquid candidates. Thermodynamic measurements and neutron scattering results will be used to analyze the coupling regime and the nature of magnetic ground state in these structurally simple but microscopically very complex materials. The presence of putative fractionalized excitations will be challenged by thermodynamic measurements in the milli-K temperature range, and prospects of reaching a genuine quantum spin liquid state in this family of compounds will be discussed.

Primary author: TSIRLIN, Alexander (University of Augsburg)

Presenter: TSIRLIN, Alexander (University of Augsburg)

Session Classification: DN2020: Plenary talks

Track Classification: DN: Plenary talks

Contribution ID: **251** Type: **Invited talk**

Impact of anisotropy on the control of spin textures

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Magnetic anisotropy does not only play a vital role in the formation and stability of long-range magnetic orders but also affects the ability to manipulate such spin structures. Via case studies, I show how competition of single-ion anisotropies at different magnetic sites can lead to unconventional magnetic orders and how modulation vectors of magnetic spirals can be controlled by tuning anisotropy.

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Session Classification: MLZ Users 2020 - Quantum Phenomena

Track Classification: UM: Quantum Phenomena

Contribution ID: **252** Type: **Plenary talk**

Studying the structural dynamics of proteins by neutron and X-ray scattering

Thursday, December 10, 2020 12:00 PM (30 minutes)

Proteins are the molecular engines of life. Their broad range of biological tasks and functions is reflected in the large diversity of specific structural and dynamical characteristics they display on broad length and time scales. A large number of experimental techniques exist that each opens a specific window onto equilibrium and non-equilibrium protein dynamics. We will illustrate, how among those, both neutron spectroscopy 1 and crystallography at XFELs and synchrotrons [2] can be carried out in a time-resolved manner to studying non-equilibrium dynamics, although on very different time scales. As to equilibrium dynamics, the combination of selective deuteration and neutron spectroscopy is particularly powerful, as will be exemplified by solvent-free protein-polymer hybrids [3] that represent one of the many interesting subjects at the interface of life sciences and soft matter.

1 Pounot, Chaaban, Fodera, Schiro, Weik, Seydel (2020) Tracking internal and global diffusive dynamics during protein aggregation by high-resolution neutron spectroscopy. *J Phys Chem Lett* 11: 6299
[2] Woodhouse, Nass Kovacs et al. (2020) Photoswitching mechanism of a fluorescent protein revealed by time-resolved crystallography and transient absorption spectroscopy. *Nature Communications* 11: 741
[3] Schirò, Fichou, Brogan, Sessions, Lohstroh, Zamponi, Schneider, Gallat, Paciaroni, Tobias, Perriman, Weik. Diffusive-like motions in a solvent free protein-polymer hybrid, *under revision*

Primary author: WEIK, martin

Presenter: WEIK, martin

Session Classification: DN2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **253** Type: **Invited talk**

Polyanion Diffusion in Polyelectrolyte Multilayers

Tuesday, December 8, 2020 1:00 PM (40 minutes)

Coatings of oppositely charged macromolecules (proteins, DNA, polyelectrolytes) are used for surface modification and functionalization. Yet, it remains a challenge to control the position and mobility of the molecules within the coating. As a model system, polyelectrolyte multilayers were used, which were prepared by the sequential adsorption of oppositely charged polyions. With neutron reflectivity, the diffusion constant of the polyanion PSS was measured. Two parameters were found to be important: (i) the conformation of the polyelectrolytes, which depends on the ion concentration in the deposition solution and (ii) the molecular weight of the polycation; the latter was the dominant parameter. Thus, the diffusion coefficient of PSS could be varied by five orders of magnitude; the observed scaling laws are consistent with sticky reptation.
An important question concerns the relationship between the polyelectrolyte composition in the multilayer and the deposition solution. Multilayers were prepared from binary mixtures of long deuterated PSS_{long} and short protonated PSS_{short}. A small amount of PSS_{long} in the deposition solution led to a disproportionate increase of PSS_{long} in the film, consistent with the higher diffusion coefficient of PSS_{short}. The results provide insight into the parameters which influence polyelectrolyte mobility and furthermore demonstrate how polyelectrolyte mobility influences film composition.

Primary author: HELM, Christiane

Presenter: HELM, Christiane

Session Classification: MLZ Users 2020 - Soft Matter

Track Classification: UM: Soft Matter

Contribution ID: **254** Type: **Plenary talk**

How much information is in my scattering data? Some recent approaches to the structure of microgels, polymers and nanoparticles.

Wednesday, December 9, 2020 11:15 AM (45 minutes)

Recent progress with soft nanostructures will be reviewed. Traditionally, data analysis follows two approaches, roughly depending on your geographic position with respect to the Rhine river. While "inversion"predominates in the east, "modeling"is more western. In short, "inversion"minimizes the use of a-priori knowledge, while modeling starts with an idea of what the structure might be, which may be wrong ⋯and fit perfectly. Of course many implementations ignoring geography have been developed, and we advocate a mixed approach based on known ingredients: e.g., assembling nanoparticles in nanocomposites, or monomers within microgels.
In polymer nanocomposites, we will show that SANS can be used to analyze the polymer interfacial region within a nm to NPs –which impacts dynamics as measured by BDS and NSE. On micron scales, thousands of NP are embedded in the polymer, and their dispersion affects both I(q) and the mechanics of the material. A statistical method based on RMC of this many-parameter problem will be presented, showing that key features like percolation can be described. Finally, the structure of core-shell microgels has been studied by SANS using deuteration. A model describing the polymer density profiles has been developed, and the surprising result is that the shell may not necessarily be where the intuition of the synthetic chemist located it. This leads to new nanostructures of striking mechanical properties, the study of which is an on-going endeavor.

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Presenter: OBERDISSE, Julian (CNRS U Montpellier)

Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **255** Type: **Plenary talk**

Update on MLZ

Wednesday, December 9, 2020 9:00 AM (30 minutes)

The MLZ directors will give an update about the MLZ during 2020 and the plans for 2021.

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Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **256** Type: **Plenary talk**

Neutron Instrumentation - Tools from Scientists for Scientists

Thursday, December 10, 2020 9:00 AM (30 minutes)

Neutron instruments are key to productive and successful experiments. Their continued development and the implementation of new ideas is the basis for enabling excellent science, increase performance of instruments or to open new fields. I will give a brief cross section of ongoing instrument developments in the Endurance program at the Institut Laue-Langevin (ILL).
In particular, recent and future advances in neutron backscattering will be highlighted. The BATS option on IN16B increases the dynamic range of the instrument by an order of magnitude and enabled the development of a new generation of high speed choppers. Currently, a 10m long neutron guide section with variable beam focusing is being implemented to enable an adaptive beam compression around the pulse chopper system.
The BATS project and several others are only possible thanks to the 'Verbundforschung' funding scheme of the German Ministry of Education and Research, which fosters strong collaboration between scientists at research centers and scientists at universities - a prerequisite for a sustainable balance between excellent instrumentation and an excellent user community.

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Session Classification: DN2020: Plenary talks

Track Classification: DN: Plenary talks

Contribution ID: **257** Type: **Plenary talk**

What has the MLZ User Committee been doing? How can it help?

Wednesday, December 9, 2020 12:00 PM (30 minutes)

This presentation will review the work of the MLZ User Committee by describing how it has been working. A short survey of the major points that have been raised will be also be presented. The major purpose of the talk will be to introduce discussions as to what users of MLZ want, and how these objectives can be helped by actions from the User Committee and MLZ.

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Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary

Contribution ID: **259** Type: **Plenary talk**

Tests of the Standard Model of Particle Physics in Neutron Beta Decay

Thursday, December 10, 2020 10:00 AM (30 minutes)

Particle Physics with neutrons addresses a number of basic and often unique questions of particle physics and cosmology at very low energies. Within the Standard Model of particle physics, neutron beta decay data serves as important input e.g. to investigate the cosmological abundance of light elements and the energy production in the Sun. Searching for new physics, precision measurements allow to test the unitarity of the CKM quark-mixing matrix and to constrain new effective couplings, as well as exotic decay modes.
In this talk, I will present recent results obtained by the PERKEO group from experiments at the ILL and discuss their implications. The follow-up instrument PERC is currently under construction at the MLZ. Its key component is a 12m long superconducting magnet system, which contains an 8m long decay volume in a novel polarisation-preserving neutron guide. PERC aims to improve measurements of several decay correlations by an order of magnitude. I will discuss its design and status.
Finally, I will present the new neutron depth profiling instrument N4DP at the PGAA beam station of the MLZ, which is an excellent example of multi-disciplinary instrument development. Nuclear reactions allow probing depth profiles of certain nuclides like ^{6}Li. The intense neutron beam, low backgrounds, and excellent energy resolution enable time-resolved in-operando studies of Li-ion batteries.

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Session Classification: DN2020: Plenary talks

Track Classification: UM: Plenary