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Seminarhaus Grainau

Book of Abstracts

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Robotics

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Embracing Digitalization for Neutron Science

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In recent years, the scientific community has witnessed an exponential growth in digitalization, presenting unprecedented opportunities for advancements in neutron science. This abstract aims to highlight the importance of embracing digitalization and incorporating cutting-edge technologies, specifically focusing on the utilization of artificial intelligence (AI) and other emerging "hot topics."

Neutron science plays a crucial role in various research areas, including materials science, chemistry, and biology. However, traditional methods for data analysis and interpretation often struggle to keep pace with the rapidly expanding volumes of data generated by modern neutron experiments. By integrating AI techniques into neutron science, researchers can unlock the potential to extract meaningful insights from vast datasets, accelerating scientific discoveries.

This talk will explore the application of AI in neutron science. Additionally, we will introduce other "hot topics" in digitalization, including data analytics, cloud computing, and high-performance computing, which can significantly enhance the efficiency and effectiveness of neutron research.

By embracing these digitalization strategies, researchers can overcome challenges, streamline workflows, and improve the accuracy and reproducibility of neutron experiments. Furthermore, we will discuss future trends and potential collaborations that can help advance the field of neutron science through digitalization.

Join us for an engaging discussion that will inspire attendees to adopt AI and other digitalization techniques, fostering innovation and opening new frontiers in neutron science.

Note: Title and abstract of this contribution were created by ChatGPT 3.5 (May 12 Version) and slightly edited by the author. Prompt: "Write an abstract of roughly 200 words for a scientific conference. The topic is 'digitalization for neutron science' and the talk will try to encourage the attendees to make more use of artificial intelligence and other 'hot topics' in digitalization."

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Hydrogen in thin films: in situ studies

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Thermal moderator-reflector design of the 24Hz target station for the High Brilliance Neutron Source

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Coupling between phonons and crystal field excitations. Old physics, new models

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Interdiffusion of polymers and water in colloids

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Contribution of Instrument control to higher throughput at instruments

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The beam time at each of the MLZ instruments is limited.
Therefore we should look around for ways to increase the
proposals running at the instruments or measure more
samples during a measurement session or perform more
scans in the same time.

All solution require a higher automation of the measurement
process. The goal has to be, give the users more
(even preliminary) results in shorter times.

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Non-trivial Spin Structures And Multiferroic Properties Of The DMI-Compound Ba2CuGe2O7

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Incommensurate spiral magnets have raised tremendous interest in recent years, mainly motivated by their wealth of spin structures with potential non-trivial topology, such as skyrmions. A second field of interest is multiferroicity: Helical spin structures are in general ferroelectric[1], enabling the coupling of the electric and magnetic properties. Both fields present enormous potential for future devices, where spin and charge degrees of freedom are coupled. Antiferromagnetic Ba2CuGe2O7, characterised by a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a material that is interesting in both of these regards and combines them with a third one: a variety of unconventional magnetic phase transitions. Ba2CuGe2O7 is an insulator characterized by a tetragonal, non-centrosymmetric space group (P-421m) with lattice parameters a = 8.466 Å and c = 5.445 Å. The main features of the magnetic structure are due to the Cu2+ ions in a square arrangement in the tetragonal (a,b) plane with dominant nearest-neighbor AF exchange along the diagonal in the (a,b) plane and much weaker FM exchange between planes, leading to a quasi-2D behaviour. Below the Néel temperature TN = 3.05K, the DMI term is responsible for a long-range incommensurate, almost AF cycloidal spin spiral with the spins (almost) confined in the (1,-1,0) plane in the ground state[2,3]. Our research is concentrated on two central aspects: At zero external field, neutron diffraction is used for a careful examination of the distribution of critical fluctuations in reciprocal space, associated with the paramagnetic to helimagnetic transition of Ba2CuGe2O7. Caused by the reduced dimensionality of Ba2CuGe2O7, a crossover from incommensurate antiferromagnetic fluctuations to 2D antiferromagnetic Heisenberg fluctuations is observed, highlighting the rich cornucopia of magnetic phase transitions in spiral magnetic textures. Recently, a new phase with a vortex-antivortex magnetic structure has been theoretically described[4]. It has been experimentally confirmed in a pocket in the phase diagram at around 2.4K and an external field along the crystalline c-axis of around 2.2T. A lack of evidence for a thermodynamic phase transition towards the paramagnet in high resolution specific heat measurements and a finite linewidth in energy and momentum of the incommensurate peaks in neutron scattering, as opposed to the cycloidal ground state, seem to mark the vortex phase as a slowly fluctuating structure at the verge of ordering. Experiments including electrical field in order to investigate its interplay with an external magnetic field are already planned and will allow for further pinning down multiferroic properties of Ba2CuGe2O7 [5].

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Complex magnetic orders and the emergent topological Hall effect in the kagome metal ErMn6Sn6

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Following the discovery of a quantum-limit magnetic Chern phase in TbMn6Sn6, the magnetic topological metal series RMn6Sn6 (R=Gd-Yb, and Y, Lu, etc.), that possesses an ideal kagome lattice of Mn, has emerged as a new platform to explore exotic states and novel functionalities. We have recently carried out the growth of high-quality single crystals of the magnetic kagome metal ErMn6Sn6, and the physical properties characterizations via the magnetic susceptibility, heat capacity, and Hall conductivity measurements. We have also undertaken comprehensive neutron diffraction experiments on both single-crystal and powder samples at the WISH diffractometer at ISIS. Our study has clearly hinted a fascinating interplay between topologically non-trivial

electronic band structures, magnetism and electronic correlations in
ErMn6Sn6.

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Short presentation of ongoing robotics projects at MLZ + Discussion

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Quench protection of high temperature superconducting magnet using metal-insulation technology

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Magnets based on high temperature superconductor (HTS) provides an extreme sample environment to provide a magnetic field to detect weaker, often diffuse signals of (quantum) disordered systems. Therefore, studying HTS magnet behavior and quench properties is an essential aspect of neutron research instrumentation. In this project, we are using metal -insulation co-winding technology, where coating a superconductor with conducting over nonconducting layer has the ability to bypass the current through resistive regions reacting to reduce the risk of quench damage. This could be one of the methods to protect the magnets from possible overheating or overvoltage conditions. In this project, we are constructing a small demonstrator HTS metal-insulated coil to study the quench behavior experimentally. For initial designing a coil, we are using finite element method (FEM) simulations to calculate magnetic fields, the magnetic forces, and the thermal management study. The demonstrator HTS coil to be tested in a standard FRM-II CCR cryostat with 80mm sample tube.

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X-ray diffraction on the charge-density wave in the kagome superconductor RbV3Sb5

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The newly discovered kagome superconductors AV3Sb5 (A=K, Rb or Cs), in which non-trivial band topology, charge-density wave (CDW), and superconductivity are intertwined, have attracted tremendous interests. Despite extensive recent investigations via X-ray diffraction and other complementary local probe techniques such as STM, NMR and muon spectroscopy etc., it remains a major challenge to gain a consistent picture about the CDW superstructure modulation wavevectors across different AV3Sb5 samples. For instance, it is rather controversial even only for CsV3Sb5 that distinct superstructure reflections in 2x2x2, or 2x2x4, or 1x1x4 types were actually observed below TCDW experimentally. The intriguing CDW fluctuations above TCDW was also found, and further clarifications are still needed. In this talk, we will present our recent single-crystal X-ray diffraction investigations, based on both in-house and synchrotron radiation facilities, of the CDW modulations over a wide temperature range in the less-studied RbV3Sb5. A unique CDW modulation of the 2x2x2 type can be confirmed for RbV3Sb5 below TCDW = 102 K, and no evidence for CDW fluctuations above TCDW could be found. Our detailed temperature dependence measurements of the CDW superstructure reflections indicate a second-order phase transition with a 2D Ising character. A comparison to other AV3Sb5 compounds and possible implications on the understanding of the nature of the CDW in these kagome superconductors will be given.

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Magnetic, electric and toroidal polarization modes describing the physical properties of crystals

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The symmetry of multiple magnetic phenomena, e.g. ferromagnetism, collinear ordering, spin reorientation, or canted antiferromagnetism, do not depend on the atomic positions. They depend only on the set of directions of magnetic moments, which we will call magnetic mode. We will present the complete classification of magnetic modes [1] based on the magnetic point groups used in two contexts: (i) the magnetic point group of the magnetic crystal class and (ii) the magnetic site symmetry point group of the Wyckoff position of interest. This classification gives restrictions to all previously mentioned phenomena [1,2]. Permutations of space inversion, $\bar{1}$, time inversion, 1', and space-and-time inversion, $\bar{1}$' allow to extend magnetic modes classification to the electric, and toroidal polarisation modes classification [3]. To highlight magnetic, electric and toroidal polarisation modes new notation of magnetic point groups was introduced [3].
Conclusion from classifications of magnetic, electric and toroidal polarisation modes is that there are multiple materials which crystal symmetry disagree with phenomena experimentally observed inside them. This gives strong motivation to re-examine their crystal structure. For instance most of the rare-earth orthoferrites, $RFeO_3$, show spin reorientation transition, e.g. $Pb'n'm(\Gamma_4) \rightarrow Pbn'm'(\Gamma_2)$ for R = Nd, Sm, Tb, Ho, Er, Tm, Yb and $Pb'n'm(\Gamma_4) \rightarrow Pbnm(\Gamma_1)$ for R = Dy, Ce. General conclusion from the continuous magnetic modes'classification is that spin reorientation is not possible within orthorhombic symmetry. The predicted monoclinic $NdFeO_3$ symmetry [1, 3] leads to a nontrivial Dirac multipoles motif which could be confirmed using neutron diffraction or resonant x-ray diffraction [4].

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Meeting challenges in the time of neutron shortage: Using complementary experimental techniques for magnetism research at the large-scale facilities

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The science community faces a challenging situation to maintain sustainable research with neutron methods at the moment. While neutron scattering is an indispensable microscopic probe for the investigations of magnetic order and spin excitations, there are complementary techniques at the large-scale facilities that are also suitable for magnetism research, such as element-specific magnetic resonant X-ray scattering at the synchrotron radiation facilities, and muon spectroscopy at the muon facilities. in this short talk, I will give an overview about our recent activities at the DNS group as well as the experience and lessons in the studies of topological and frustrated quantum magnets using these complementary experimental techniques at various synchrotron radiation and muon facilities in the world, with the emphasis on their unique strengths as well as their complementarities to neutron scattering.

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Particle physics

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Additive manufacturing of custom neutron shielding solutions

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Together with ColorFabb we developed a 3D printable shielding material based on PLA and hexagonal boron nitride, allowing to easily manufacture complex shielding geometries, even with hobby-grade 3D printers. While using the material we have seen considerable interest internally, as well as from external collaboraters, and gained experience in designing and printing custom shielding solutions. Hence, we would like to share our experience in working with the material and discuss further developments.

Parallel 2 / **22**

Data management as MLZ - future perspectives

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This contribution will give a short overview on the plans for data management at MLZ - i.e. the workflow from proposal, epxeriment, storage, visualisation to analysis and publication. This contribution is thought as brief introduction to the further discussion on requirements from the instrument scientists perspective.

Parallel 2 / 2

Monte-Carlo simulations of the new radiation shielding at the thermal beamport SR8 @ FRM II with SERPENT 2

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The thermal beamport SR8 at the research neutron source Heinz Maier-Leibnitz in Garching will be optimized to allow the simultaneous operation of three independent monochromatic powder diffractometers. SPODI will continue to be one of the world-leading high-resolution powder diffractometers. FIREPOD will be a dedicated high throughput instrument, well suited for a broad range of fast parametric studies. ERWIN will be a highly versatile multi purpose diffractometer for both powder as well as single crystals. Due to the unique characteristics of each instrument, the optimized beamport SR8 will be able to cater for a wide range of experimental demands and will substantially increase available beam time for neutron powder diffraction. To exploit the full capabilities of each instrument a complete rebuilt of the primary neutron optics at the beamport SR8 is necessary. This requires an entirely new radiation shielding around the neutron guides and monochromators.

In this contribution, the results from detailed Monte-Carlo simulations to optimize the biological SR8-shielding are presented. Employing the SERPENT2 code, the full radiation transport of neutrons, as well as gamma radiation through the different shielding materials is simulated. While taking boundary conditions such as available space, floor load and costs into consideration, the underlying detailed CAD-based model is iteratively optimized to achieve a total dose rate lower than the desired limit of 3μSv/h outside the shielding.

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Activities of the Data-Driven Discovery Group on Data Reduction for MLZ Instruments

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Data reduction is a transformation of a dataset collected during a scattering experiment into a dataset in physical units. It requires detailed knowledge of geometry and configuration of the instrument at which the dataset was collected. As a result, data reduction is an essential stage required for linking raw experimental data to a meaningful scientific publication. As such, development of automated and user-friendly data reduction workflows for MLZ instruments is among main foci of the Data-Driven Discovery group. In my talk, I will discuss our recent activities in this context, including: a) development of graphical user interfaces for the DNS and POWTEX instruments, b) integration of the data reduction workflow for SANS-1 into the popular Mantid [1] framework, c) inclusion of multiple scattering into analysis of polarized neutron diffraction data.

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Development of in-situ techniques for neutron scattering instruments or: How to mitigate the negative effects of (future) reactor shutdown periods at MLZ.

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Let us face it: The research reactor FRM II will experience future shutdown periods of 6 months or longer also in the near and far future be it due to regulatory issues with the local government or be it due to technical problems encountered. In this contribution I would like to show how to mitigate the negative effects of these shutdown periods and to turn them into something productive and positive for the whole MLZ.
First, I will dwell upon the recent developments of in-situ techniques at neutron scattering instruments which were performed at the MLZ. I will also summarize the new sample environment options developed, as far as I have learned about them. The latter lists will not be complete, since I do not aim to demonstrate what we have done in the past, but I would rather look into the future: What can we do and develop together with user groups in the future using the time and staff available due to the (future) reactor shutdown periods.
I will also quickly summarize the new facilities in the surrounding labs made available for users recently.
To transfer these efforts to politicians and research budget holders I suggest to bundle the above mentioned activities and to give them a common name and web-page design visible to outside users and scientists even at the early stage of a first drawing or idea. This might enable more user groups to join the efforts on site and it might open up routes to write common grant proposals. Especially in light of the up-coming sources, the European Spallation Neutron Source (ESS) in Lund or a high brilliant neutron source (HBS) in Jülich, one should position the MLZ as a knowledge base for not only neutron instrumentation, but also sample environment and in-situ techniques.
In the past, the Helmholtz Zentrum Berlin has demonstrated a similar concept with great success despite being a neutron source with a somewhat smaller reactor power.

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Development of a Nested Mirror Optic Array for the Thermal TAS PUMA at MLZ

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A persistent challenge for the inelastic neutron scattering technique has been the low scattering cross-section of neutrons, necessitating large sample sizes compared to elastic neutron scattering or inelastic x-ray scattering. Focusing the neutron beam is a viable technique to increase the flux reaching the sample, but previous techniques suffer from limitations to beam size, beam quality or an excessively close distance to the sample which interferes with sample environments. The nested

mirror optic (NMO) is an ideal solution in many ways to overcome these challenges and provide a small, well-behaved beam at the sample position while keeping the optical components a reasonable distance to make room for the sample environment equipment. An ongoing project has led to the development of an NMO prototype for the cold triple-axis spectrometer (TAS) MIRA at MLZ, but with a limited energy transfer range. The development of supermirror coatings with large m-values has opened up the possibility to apply this technique to the thermal TAS instrument PUMA at MLZ. While current focusing techniques on PUMA yield a cross section of 20mm x 20mm, the current NMO project seeks to develop, install and commission an NMO setup that will reduce the beam size to 5 mm x 5 mm while preserving 50% of the incoming neutrons, for an 8-fold increase in flux on small samples. It will do this while also providing space for the sample environment and preserving the beam characteristics, and will be straightforward to mount and dismount to adjust for the needs of each user. I will discuss the planned setup and our current progress in designing the NMO setup for PUMA, as well as the scientific case for such a device with several planned use cases.

Parallel 2 / **13**

HYMN –A novel unified toolbox for in-situ magnetic hyperthermia experiments using neutron scattering

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One of the most promising use cases of magnetic hyperthermia, is the use of magnetic nanoparticles (MNPs) for cancer therapy. In this treatment, MNPs are immersed into tumours and by heating with external magnetic fields, typically 100-900 kHz, destroy cancer cells. Since it is a clinical application the optimization of field parameters and in turn, the heating power, is crucial to maintain both safety and high efficiency. Safety dictates an upper limit of applied magnetic field exists. Hence, for successful application, the heating power needs to be improved by the optimization of MNPs structure. What is more, recent studies have shown a huge increase in magnetic heating by the excitation of transversal spin modes in MNPs, in low GHz range. An ideal tool for the characterization of such MNPs is small angle neutron scattering (SANS), with the extended functionality provided by the MIEZE technique. The aim of our ERUM-Pro HYMN project is to develop a novel, unified experimental and computational toolbox for in-situ magnetic hyperthermia experiments under clinical conditions, utilising the SANS and MIEZE-SANS technique, combined with nanomagnetic simulations. This will be achieved by the development of two custom-made setups for operation in the 100-450 kHz (up to 30 mT) as well as 0.5-4 GHz (up to 2 mT) range. We present first SANS results, where we used in-situ RF heating at 450 kHz to examine the dynamic structure formation of magnetite nanocubes with 12, 34 and 53 nm size.

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Discussion

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Preparation of a CaBER Sample Environment and Microfluidic Devices for In-Situ Scattering Measures of Polymer Solutions in

Extensional Flow

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Microfluidic flows using hyperbolic contractions and capillary break-up extensional rheometery (CaBER) have emerged as key techniques to characterize polymer solutions experiencing uniaxial extensional flow [1,2]. In this work, two approaches are presented to explore the microstructural evolution during extensional flows and relate those features in situ to the macroscopic properties exhibited by polymer solutions during extension. A CaBER sample environment has been prepared for use at small angle scattering (SAS) beamlines to conduct simultaneous CaBER-SAS experiments by configuring the instrument such that the beamline, linear motor, and high-speed camera are perpendicular to one another. An essential feature of the setup is a novel geometry and sample cell to allow for repeated testing of a single polymer solution sample by limiting effects such as solvent evaporation and inconsistent (re)loading conditions. As a second approach a multi-channel microfluidic device has been prepared. The channel profiles resemble hyperbolic contractions and have been manufactured through selective laser etching by. To allow for microstructural characterization in situ the channels within the microfluidic device have been arranged in a 2D array, increasing the overall effective volume of material within the device, and ensuring sufficient signal in a SANS environment. Solutions of 35 kDa and 8 MDa PEO in water with concentrations in the dilute and semi-dilute regimes have been tested in both devices to determine the setup's efficiencies during repeated testing in the CaBER environment as well as to characterize the flow profile within the stacked microfluidic device.

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Status of the On-Site High Pressure Diffraction Option on Single Crystals at MLZ

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The neutron single crystal diffractometer HEiDi uses the hot source of FRM II to offer high flux down to short wavelengths. Its large q range and flexibility concerning experiments between 2.5 K and 1300 K make it a versatile tool for detailed studies on structures for many topics in physics, chemistry and mineralogy.
In two consecutive BMBF-funded projects from 2016 to 2022 (05K16PA3, 05K19PA2), the application

suite of HEiDi (and its polarized twin POLI) was extended to enable high-pressure (HP) experiments, firstly with diamond anvil cells [1, 2] and recently by introducing clamp cells for larger sample volumes [3]. These cells can also be used on DNS and MIRA to perform comprehensive experiments on shared samples/PCs.
This overview presents the status of the various new HP cells and their possible applications as well as some related technical developments in neutron optics at HEiDi, for instance a new 2D PSD currently under construction. These extensions will increase the instruments performance not only for HP experiments and thus open up further applications as well.

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New laser furnace for the STRESS-SPEC instrument

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Current topics in materials research such as new production processes, e.g. additive manufacturing (AM), or sustainable energy research, e.g. high-temperature alloys, require a highly flexible sample positioning system during diffraction experiments. Therefore, the STRESS-SPEC group has pioneered the use of industrial robots for sample handling and positioning at neutron diffractometers [1, 2]. To fully exploit the capabilities of the robotic positioning system, a dedicated sample environment is essential. In this talk, we will present a recently developed lightweight laser furnace with a large neutron acceptance angle, which allows the investigation of samples at elevated temperatures up to 1100 ℃, while benefiting from the positioning flexibility of a 6-axis industrial robot. The furnace control rack was built with interoperability in mind, allowing to control various other sample environment devices as well. Some features and example use cases of the laser furnace will be presented.
Furthermore, we will also give an outlook at the future development of a lightweight mechanical tensile testing machine that can also be mounted on a 6-axis industrial robot.

[1] H.-G. Brokmeier et al., Mater. Sci. For. 652 (2010) pp. 197–201. DOI: 10.4028/www.scientific.net/MSF.652.197
[2] C. Randau et al., Nucl. Instr. Meth. A 794 (2015) pp. 67–75. DOI: 10.1016/j.nima.2015.05.014

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Discussion

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Magnetic Neutron Scattering –From basic scattering theory to cutting edge applications

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Since their inception, neutron scattering methods have significantly contributed to many advancements in solid state research. This is especially true for the study of magnetic materials, where neutrons provide a uniquely qualified probe to investigate magnetism on the microscopic scale. This talk aims to elucidate the relation between the magnetic properties of a sample and the observable neutron scattering cross sections. Contemporary examples, will be used to connect the basic theory with real world measurement data acquired at a variety of instruments like small angle scattering, single crystal and powder diffraction, three-axis spectroscopy as well as neutron imaging. Finally, a deeper dive into low-dimensional magnetism in metal-organic compounds will showcase the connection of solid state magnetism and sought-after phenomena such as quantum criticality and high temperature superconductivity. This will highlight the importance of magnetic neutron scattering in condensed matter physics and material science.

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Hydrogenation change magnetism in nm thin film

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Unknown structure solving and its further application combined with the theoretical simulation

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Neutron imaging at MLZ

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Current neutron detection techniques for neutron scattering applications - Overview and perspectives

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The advent of the new spallation sources as well as the various major upgrade programmes of existing facilities have given great impetus to the new and further development of neutron detection techniques for neutron scattering applications in the last decade. Great progress has been made, particularly in the area of count rate capability and large detection areas.
With regard to the projects planned as part of the MORIS program, this presentation is intended to give an overview of the current technologies, their performance, strengths and weaknesses and perspectives

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Electrodepositing lithiophilic nanoparticles as artificial interphase for anode-free lithium ion batteries

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Anode free batteries are designed to significantly decreases the weight of a cell.They necessitate immaculate reversibility of the charge
and discharge process, as no further lithium other than the amount loaded into the cathode is available. Homogeneous plating and
stripping of lithium onto a current collector is not readily achieved when plating on e.g. on copper. Lithiophilic metals like Au and Zn
can be used to engineer the surface of a current collector, for example through the application of a thin sputtered film (50 nm), with
which the lithium forms metallic interphases and hence drastically changes the plating environment. This can be explored further through
the electrodeposition of said metals, which can be generated with different size and number density and therefore provide a variety of
plating substrate configuration. Correlating morphology and arrangement of the particles to their electrochemical behaviour in lithium half cells should elucidate their effect on the anode interphase and allow for precise decoration of the current collector for improved batteries.

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Topology correlation to nanoscale hydration of polymer brushes

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By utilizing time-of-flight neutron reflectometry (ToF-NR) under different relative humidity, we demonstrate that polymer brushes constituted by hydrophilic cyclic macromolecules exhibit more compact conformation with lower roughness compared to linear brush analogues, due to the absence of dangling chain ends extending at the interface. [1] In addition, due to increased interchain steric repulsions, cyclic brushes feature larger swelling ratio and increased solvent uptake with respect to their linear counterparts presenting the same composition and comparable molar mass. Moreover, the two topologies exhibit differences in ageing, upon repetitive cycling/drying trials.
To correlate the equilibrium swelling ratios as a function of relative humidity for different topologies a new form of the Flory-like expression for equilibrium thicknesses is proposed. The relative humidity represents the chemical potential balance between brush and surrounding environment. The Flory-like expression, which has been utilized so far for thin polymer films, breaks down for the cyclic brush. Additional topological contributions need to be taken into account in this expression, in order to rationalize differences reflected in swelling ratios and solvent content between the linear and cyclic polymer brush topologies.

[1] Vagias, A., Nelson, A., Wang, P., Reitenbach, J., Geiger, C., Kreuzer, L. P., Saerbeck, T., Cubitt, R., Benetti, E. M., Müller-Buschbaum, P., The Topology of Polymer Brushes Determines Their Nanoscale Hydration. Macromol. Rapid Commun. 2023, 2300035

Parallel 4 / 7

Diffusion of water in waterborne polymer colloid films containing different hydrophilic shells

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The waterborne latex films, obtained from the dispersions of latex particles are of particular interest due to the non-content of volatile organic compounds (VOC), which is often mandatory under environmental legislation [1]. However, abrupt water penetration inside the films restricting their lifespan and deteriorating the shining of the coating, limiting their uses [2]. In order to prepare efficient and solvent-free coatings with the low glass-transition temperature (Tg < the drying temperature) but with higher mechanical strength, we have integrated hydrophilic layers (Acrylic acid/ Poly(acrylamide)) around the hydrophobic cores (mixture of Methyl methacrylate and Mutyl acrylate) in the latex film. Polymer latex particles with different morphologies (hairy layer variants and core-shell particles) have been synthesized using emulsion polymerization. Polymer latex films have been prepared in the next step by evaporating water in a thermo- and humidistatic chamber at temperature 25 oC. The structure formation of polymer latex films in the dry state (crystallinity) and in

re-swelled state (change in crystallinity and whitening or blushing) have been studied to propose a recipe for the preparation of efficient latex coatings. The combine study by small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) show the FCC-like structure formation by the latex film, which become more organized with the inclusion of the that the hydrophilic shell. The inclusion of hydrophilic shell also promotes the formation of the homogeneously swollen film and slows down the development of water "pockets", preventing the deterioration of the latex film over time.

1. T.N. Tran, E. Rawstron, E. Bourgeat-Lami, D. Montarnal, ACS Macro Lett. 7 (2018) 376.
2. I. Konko, S. Guriyanova, V. Boyko, L. Sun, D. Liu, B. Reck, Y. Men, Langmuir. 35 (2019) 6075.

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Thermal and structural behavior of graphite battery anodes

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High-performance graphite evolved to the most common anode material and is used in nearly every commercial Li-ion battery nowadays. However, there is a clear lack of information about the structural stability of Li_xC_6 and its phase diagram. In literature, temperature-resolved phase stability of lithiated graphites is therefore studied poorly and the results are often controversial. Hence, the structural evolution of lithiated graphites was studied at high temperatures showing the decomposition of the lithiated anode and a corresponding loss of intercalated lithium ions, resulting in the evolution of phases like LiF and Li_2O, which are strongly correlated with the degradation of the solid electrolyte interface (SEI).

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A new type of redshift - investigation of CsCaHxF3−x:Eu2+

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The heteroanionic approach for the design of materials has led to variety of novel systems with unique properties. In particular, heteroanionic hydrides emerged with promising properties themselves. Over the recent years such compounds, in particular hydride fluorides have been thoroughly investigated as potential host materials for rare earth activated luminescence.
Here, the solid-solution CsCaHxF3−x:Eu2+ is presented as the first calcium containing system of this kind. Investigations of the solid-solution's properties reveals unique optical behaviour: by increasing the hydride content within the series, a completely new type of redshift is observed upon excitation with UV-light. Instead of a single red-shifting emission band, new narrow emission bands emerge at the low energy regions. In total, the ratios of these emission bands determine the observable emission colour. Such a redshift mechanism has not been reported for any related system.
For the elucidation of this behaviour, a variety of analytical methods were applied. With the help of neutron diffraction data, obtained at the SPODI@MLZ, in combination with X-ray diffraction data, the crystal structures were fully solved. Further analytical techniques such as luminescence spectroscopy and vibrational spectroscopy then allow for the full understanding of this unique behaviour which will be explained in detail herein.
These findings will help for the design for new efficient phosphors, especially useful for red-emitting pc-LEDs.

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Electric Field-Induced Assembly of Highly Crosslinked Ionic Microgels

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The electric field driven assembly of highly crosslinked ionic microgels at effective volume fraction, ϕeff=0.04 is studied using a confocal microscope. The isotropic microgels undergo structural transitions depending on the field strength and microgel concentration. At low ϕeff, the ionic microgels interact via long-range Yukawa type interaction and the interparticle separation between microgel particles is much larger than the microgel particle diameter. Each microgel particle experiencing the field can be considered as a point dipole. These point dipoles are attracted mutually and assemble along the direction of the applied field and align to form linear chains. At a higher field strength, a gas phase co-existing with islands of a bct and ring structures are observed in the xy plane. Clusters with fewer microgels tend to form rings, whereas larger clusters arrange into bct structure. The microgels instantaneously redisperses once the electric field is turned off.

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Recent instrument development and plan on POLI

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The single crystal diffractometer POLI is dedicated to diffraction using polarized neutrons and can additionally host bulky sample environments. Currently, three standard setups are implemented on POLI: zero-field spherical neutron polarimetry, flipping ratio method with high magnetic fields and non-polarized diffraction under various special conditions. Here we reported our recently instrument developments, including an 8T magnet with very low stray fields, a supermirror bender polarizer, SEOP polarizer and analyzer, piezo-driven slits and new incident wavelengths. We will also present our detector upgrade plan related to the BIDIM detector from LLB and the proposal in the MORIS program.

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Event Mode Neutron Imaging Detectors

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Event mode neutron imaging detectors generate information for every neutron hitting the detector individually. This allows the usage of algorithms to analyze the individual events and improveme noise supression as well as temporal and spatial resolution. The detector have already been tested sucessfully for fast, thermal and cold (ToF) imaging, and neutron diffraction.

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The Study of Local and Higher Order Structure in Soft-Matter Systems by Contrast-Variation Simultaneous SANS & WANS

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Materials based on semi-crystalline polymers are used in different fields of applications, from high temperature to plastics, elastomers and fibers, from biomedicine to aerospace, from oil industry to fuel cells. Such materials exhibit a phase separation in crystalline and amorphous regions. The crystalline domains are characterised by a complex morphology spanning a broad length scale from Å to hundreds of micrometres and consisting of hierarchically organised, multiple structural planes such as crystalline unit cells, lamellar crystals, fibrils or boards and fibres or spherulites. Furthermore, the amorphous regions in the bulk and between the lamellae can be functionalised, leading to even more complex morphologies when external stimuli such as humidity (RH), temperature (T) or uni-axial deformation (UD) are applied to the sample. For the structural characterisation of such complex morphologies, a large length scale has to be covered, which usually requires a combination of different experimental methods in structural analysis. Due to the advantage of contrast variation and the large Q-range that can be covered, small angle (SANS) and wide angle (WANS) neutron scattering techniques are particularly suitable for the detailed study of natural and synthetic polymeric materials. However, when working with different instruments to collect scattering data in wide and small scattering ranges, it is difficult to ensure perfect reproducibility of sample composition and quality as well as external field conditions so that a global analysis of data collected in different experimental geometries and at different times can be reliably performed. The simultaneous use of wide and small neutron scattering methods in the same experiment is therefore necessary for sensitive or expensive samples when special care must be taken with sample preparation (composition, quality, quantity, etc.) or treatment (temperature, humidity, etc.) during the experimental investigation.
Here I report on the experimental investigation of various semi-crystalline polymer and soft-matter systems under different RH, T and UD conditions using neutrons on pinhole SANS or TOF SANS/WANS diffractometers, with emphasis on the Q range and experimental resolution involved in structural studies. The use of complementary methods (SAXS, FTIR, etc.) to better understand the local or long-range structures will also be discussed.

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Structure evolution in LNMO, a novel cathode material for Li-ion batteries

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High voltage spinel LNMO is one of the most promising next-generation cobalt-free cathode materials for Li-ion batteries. Besides the typical compositional range of LixNi0.5Mn1.5O4 (0 < x < 1) in the voltage window 4.90 to 3.00 V, additional Li can be introduced into the structure in an extended voltage range to 1.50 V. Theoretically, this leads to significant increase of the specific energy from 690 to 1190 Wh/kg. However, utilization of the extended potential window leads to rapid capacity fading, voltage polarization that lack a comprehensive explanation.

In this work, we conducted operando XRD and neutron diffraction on the ordered stoichiometric spinel LixNi0.5Mn1.5O4 within 0 < x < 2.5 in order to understand the dynamic structure evolution and correlate it with the voltage profile [1]. We were able to provide a conclusive explanation for the additional voltage step at 2.10 V, the sloping voltage profile below 1.80 V, and the additional voltage step at ~3.80 V.

[1] Nicola M. Jobst, Neelima Paul, Premysl Beran, Marilena Mancini, Ralph Gilles,Margret Wohlfahrt-Mehrens, and Peter Axmann, J. Am. Chem. Soc. 2023, 145, 4450–4461

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Event-based neutron radiography with Image Intensifier and CMOS camera

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High-resolution neutron radiography requires an imaging system capable of detecting the exact location of the absorbed neutrons in the scintillator screen. This is realized by a sensitive CMOS camera with high frame rate capabilities and an image intensifier, which is able to amplify the weak light output created by individually absorbed neutrons. Identifying and recording single neutron events appearing as a cluster of intensity spots allows narrowing the point spread function of the imaging system compared to conventional intensity-integrated detection mechanisms. Further, it facilitates the characterization and optimization of the scintillator properties for better imaging performance.

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Interaction of nanoparticles with lipid films: the role of symmetry and shape anisotropy

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Nanoparticles are nowadays widely used in biology and have quickly emerged as essential to modern medicine. When nanomaterials come into contact with biological membrane, their interaction with biomacromolacules and biological barriers will determine their bioactivity, biological fate and cytotoxicity. It goes without saying that understanding the interaction between nanomaterial and biological interfaces is vital to bridge the gap between design/synthesis/engineering of nanoparticles and their full translation into end-use applications. In this context, the role of symmetry/shape anisotropy of both the nanomaterials and biological interfaces in their mutual interaction, is a relatively unaddressed issue.
Here we present the findings about the interaction of gold nanoparticles (NPs) of different shape, i.e. nanospheres and nanorods, with biomimetic membranes of different symmetry, i.e. lamellar (of 2D symmetry), and cubic (of 3D symmetry) membranes.
Through the combination of structural scattering techniques (in particular Neutron Reflectometry), we observed that, on a nanometric lengthscale, the structural stability of the membrane towards NPs is dependent on the topological characteristic of the lipid assembly and of the NPs, with higher symmetry related to higher stability. Moreover, Confocal Microscopy analyses highlight, on a micrometric lengthscale, that cubic and lamellar phases interact with NPs according to two distinct mechanisms, related to the different structures of lipid assemblies.
This study represents a first attempt to systematically study the role of membrane symmetry on the interaction with NPs; the results will contribute to improve the fundamental knowledge on nano-bio interfaces and, more in general, will provide new insights on the biological function of lipid polymorphism in interfacial membranes as a response strategy.

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CGO-Cu cermets characterization by in situ scattering measurements with a dilatometer

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The long-term stability of solid oxide fuel cells (SOFC), electrolyzers (SOEC) and catalytic membrane reactors is highly dependent not only on their electrochemical properties but also on the similar thermal evolution of all their constituting parts, ensuring mechanical compatibility, i.e. electrolyte and electrodes. This kind of devices have a good performance at high temperatures. However, high temperatures and thermal cycling put strain on cell constituents, and oxidation of electrodes caused by demixing of fuels and water limit both operation and lifetime. Thus, the decrease in operation temperature is needed. Most SOFCs are based on yttrium-stabilized zirconia (YSZ) electrolyte, between a porous Ni/YSZ anode and a porous lanthanum strontium manganite cathode, which operate above 800 ℃. In order to decrease the operation temperature of these devices new electrolyte materials are under study. $Ce_{0.8}Gd_{0.2}O_{2-\delta}$ (CGO) is an ionic conductor capable to operate at 600-800 ℃, whose performance improves by decreasing thickness. Therefore, there is a need of finding compatible anode materials with enough electronic conductivity and electrocatalytic activity that are also mechanically stable to support the thin electrolyte. Cu based ceria cermets demonstrated to be advantageous in replacing Ni-cermets for the direct oxidation of hydrocarbons since, unlike Ni-containing cermets, Cu does not promote significant carbon coking. In these cermets the electrical conductivity is warranted by Cu, whereas ceria is responsible for the catalytic activity in oxidation reactions, partially compensating the Ni catalytic activity in standard Ni-YSZ electrodes. Besides, Cu is more economically viable than Ni.
In this study, we optimized CGO-Cu composites as anode materials for CGO electrolytes. Different

samples with different ratios of CGO and Cu ranging from 40-60 to 70-30 vol.% were studied by high temperature in situ x-ray diffraction (XRD @P07 Desy) at the same time as the dilatometric signal was obtained. Differences in the micro (XRD) and macro (dilatometer) thermal expansion coefficient (TEC) due to the different ratios of the composites were correlated with the microstructure (SEM and XRD) and with the electrochemical properties, which allowed selecting best anode materials for high temperature green energy applications.

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Defect Studies in Tungsten using Positron Annihilation Spectroscopy

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We study vacancy-type defects in tungsten mono-crystals using positron annihilation Doppler-broadening and lifetime spectroscopy. These studies are part of nuclear fusion research necessary to predict the durability of reactor walls.

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Diskussion

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Sassena – a tool for validation of Molecular Dynamics simulations with neutron and X-Ray scattering experiments

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Neutron and X-ray scattering experiments are powerful techniques to investigate any material at the atomic to mesoscopic level. They give us structural and dynamic information. However, it is not possible to extract the relative position, shape, and velocity of the scatterers directly from the scattering data due to the phase problem. One possibility to circumvent this problem is to simulate the materials at different length scales and to calculate scattering patterns from these simulations.
To cover the several orders of magnitude in reciprocal space accessible by scattering techniques, a high-performance software solution is required to deal with large systems at fine resolution. For

this task, several programs are available; we have chosen Sassena for our work. Sassena inherits distributed memory parallelization (MPI) from its previous version. We augmented this by vectorization and shared memory parallelization (OpenMP) to bolster the computing speed; gains of up to an order of magnitude were achieved. Furthermore, the introduction of shared memory parallelization introduces the possibility of hybrid parallelization.

Additionally, we also added a new feature in the program that allows the removal of the coherent scattering signal caused by the finite size of the simulation box.

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Revealing nature's secrets with the Higgs boson

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Plenary 4 / 56

Towards an improved understanding of food emulsions via neutron scattering and neutron spectroscopy

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The stability of food emulsions depends -beside other effects- on a complex interplay between proteins, phospholipids, oil and water. Preparing milk-based and sustainable plant-based emulsions requires good knowledge in interfacial and emulsion stabilization mechanisms, affected by the emulsion composition. To understand these mechanisms in detail different length scales from interatomic to macroscopic distances need to be investigated.
Neutron scattering techniques provide insight into such emulsions on these length scales depending

on the technique used. Combining structural information on molecular length scales from small angle x-ray and neutron scattering (SAXS and SANS) with time dependent neutron spin echo spectroscopy (NSE) allows to expand our understanding towards intermolecular interactions within the interface. These interactions are linked to the emulsion stability –the elastic properties of the protein or protein/phospholipid stabilized oil/water interface on molecular length scales. NSE provides in this combination the time dependent correlation function in reciprocal space, S(q,t), on molecular length scales and time scales in the nanosecond range relevant for thermally driven motion of mesoscopic systems such as the emulsion interfaces.
This presentation introduces the neutron and x-ray scattering techniques which broadens the classical characterization of food emulsions. Results from emulsions stabilized with β-lactoglobulin as a representative milk protein, and different plant-based proteins, are presented and discussed. Contrast variation by deuteration of some components of the emulsions is applied to focus on the interfacial region, relying on the uniqueness of neutrons.
Connecting these emerging results with classical characterizations such as interfacial tension or viscoelasticity helps understanding the complex mechanisms of interfacial stability and may contribute to a knowledge driven development of sustainable food emulsions.

Parallel 5 / 4

Elasto-plastic behaviour in titanium alloys

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Neutron and synchrotron diffraction studies under mechanical stress in titanium alloys Ti-64 (near α-alloy), Ti-6246 (α+β alloy), Ti-5553 (near β-alloy) and Ti-38644 (β-alloy) were performed to investigate the deformation mechanisms. In particular, the determination of single-crystalline elastic constants derived from the measured lattice strains in the polycrystalline specimens will be presented. These results have been used further to quantify the load partitioning in the elastic regime between the softer bphase and stiffer aphase. In addition, diffraction data were collected along the entire elastic and plastic regime to determine the evolution of lattice strains, texture and phase compositions.

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Diffraction computed tomography and its applications

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Attenuation-based radiography and tomography (CT) are well-established experimental techniques for non-destructive visualisation of the object interior, where X-/gamma-rays and neutrons are most commonly used types of the incident radiation, but also protons or heavy particles (e.g. ions) can be used as a source. Different radiation sources are used along with phase-contrast, Bragg and/or energy-selective imaging for gathering complementary information enabling the enhancement of contrast and sensitivity beyond the limitations of X-rays.
Alternative way to increase sensitivity to density variations and chemical composition as well as to improve the discrimination of chemically and morphologically similar, but structurally distinct phases is the accounting for scattering effects in the radiography and tomography. This pawed the way to diffraction CT –an experimental technique combining diffraction with Computed Tomography in the form of either XRD-CT or ND-CT, where similar to traditional CT, the sample is scanned

by a pencil-beam, but the diffraction picture is collected instead of the attenuation pattern in the transmitted beam. Prominent progress has been achieved during the last decades in increasing spatial and temporal resolution especially for studies of energy materials, biological samples, catalysts, fuel cells etc.
In the current contribution we report the applications of diffraction-CT to studies of lithium distribution in commercial cylinder-type Li-ion batteries as well as the implementation and first results of ND-CT (Neutron Diffraction with Computed Tomography) experiments using monochromatic thermal neutrons.

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Polysaccharide-based nano-/micro-gels for the food sector

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Polysaccharides are the major natural originated components finding extensive investigation and utilization in diverse fields including the nutritional manufacturing sector. Due to their advantageous properties such as safety, stability, biocompatibility, biodegradability and nontoxicity, polysaccharide-based complex systems have a significant potential in the fields of cosmetics, pharmaceutics and food engineering. Microencapsulation of active ingredients such as, flavors, antioxidants, vitamins, lipids into biopolymer nano-/micro-gels offers greater bioavailability, effectiveness, lower toxicity and more lasting stability than conventional formulations. Understanding the physicochemical properties of these micro- and nanogels and their encapsulating and release properties in different conditions is therefore crucial for their optimization and use in the food sector.
In this communication we present k-carrageenan-based nanogels obtained as a result of coassembly with a-lactalbumin as macro-ionic crosslinking agent. Such systems are of interest as carriers for bioactive ingredients therefore we compared the microstructure and VD3 encapsulation capacity of nanogels as a function of preparation protocol and various environment conditions (pH, T) applying combination of scattering and spectroscopic techniques.

Parallel 5 / 14

How is the biological effect of fast neutrons on human tissue mediated?

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In fast neutron therapy with a fission beam, damage to irradiated cells is mainly due to secondary protons and electrons from neutron and gamma interactions, respectively. For the severity of biological effects on cells and the DNA in particular, the occurrence of interaction clusters plays a crucial role. The occurrence of clustered damage differs for neutron and gamma radiation which is reflected in both the application of neutrons in external radiotherapy and the risk evaluation in radiation protection.

Parallel 5 / 1

Lamella orientation control of β-Solidifying TNM Alloys via High-Temperature Compression

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The third generation β-solidifying TNM alloys with (α2+γ) lamellar microstructures have been considered excellent candidates for modern turbine blades due to their low density, high specific strength and stiffness, excellent creep resistance, and good corrosion resistance. It has been found that orienting the γ lamellae to the direction of the load can significantly increase the mechanical properties of the alloys, making lamella orientation control (texturization) an interesting topic for property optimization [1].
In this study, high-temperature compression (with a dilatometer) was first achieved to texturize the alpha phase through optimization of compressive speed and strain. An optimum fiber texture for the alpha phase has been identified by combining EBSD analysis with an in-situ XRD synchrotron.
Moreover, experiments were performed to observe the effect of the strain rates, taking a high strain rate of 1 s-1 and low strain rate of 10-2 s-1 while keeping the other parameters constant (cooling rates, externally applied load during cooling, total deformation, and temperature). A difference in behavior for the true stress-strain curve has been highlighted corresponding to a different type of mechanisms of dynamic recrystallization.
Our results show that the microstructure and texture of TiAl alloys can be effectively controlled, and it seems that having a high deformation and a low strain rate should promote the uniform fiber texture.
Further analyses are needed to understand the mechanisms behind the observed texture evolution. These findings have potential implications for optimizing the processing and performance of TiAl alloys.

[1] « Polysynthetic twinned TiAl single crystals for high-temperature applications » Chen et al. Nature Materials vol.15 August 2016

Parallel 5 / **24**

Why elemental analysis is important in neutron scattering centers?

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Elemental analysis with neutrons is based on the excitation of atomic nucleus inducing penetrant gamma rays, thus enabling the non-destructive bulk analysis of samples. With prompt gamma activation analysis (PGAA), all elements can be detected: the higher their neutron capture cross section, the stronger their signal in the gamma spectrum. It is unique in the determination of light elements (like H, B, also D), as well as in the characterization of neutron shielding.
We have received many inquiries regarding neutron activation analysis (NAA), our new instrument, as it is still one of the most sensitive method for trace elements (Co, Mn, Na, etc.), and is also important in the determination of activating nuclides in structural components.
PGAA has continuously been developed during the past 15 years with lowering the spectral background, with introducing new 64k digital spectrometers of great potential. We have introduced a

low-background counting chamber for determining short-lived beam-activated nuclides. PGAA now also accommodates Neutron Depth Profiling with world-class characteristics.
We have more ambitious plans for the future: we want to detect all (detectable) particles induced by neutrons to reach a broader circle of elements with higher sensitivities (e.g., P in Si, Pb in bronzes, etc.). The combination of the methods (PGAA+NAA, short-cyclic NAA, PGAA+NDP, PGAA+imaging) open new directions, to which our user community is looking forward.

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Effect of Amyloid-β(1-42)-Monomer and protofibrils on dynamics of brain phospholipid liposomes and the Aggregation Kinetics Amyloid-β(1-42)

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The cognitive dysfunctionality stems from Amyloid Aβ (1-42), a neurotoxic peptide which is primarily responsible for Alzheimer's disease and is predominantly found in the extracellular spaces in the form of senile plaques. Aβ42 has a strong propensity to interact with the phospholipid membrane, sphingomyelin, ganglioside GM1, and cholesterol. The plasma membrane is the first biological building block encountered by the Aβ42. Hence, the impact of Aβ42 on the structure and dynamics of the brain phospholipid membrane is important to understand Aβ42 pathogenesis. Furthermore, the aggregation kinetics of Aβ42 in presence of brain phospholipids is of prime interest due neurotoxic behaviour of the Aβ42. We have prepared 100 nm unilamellar vesicles from the brain phospholipids which are mainly composed of phospholipids and sphingomyelin extracted from the porcine brain tissues. Moreover, we have prepared different aggregation states of Aβ42-monomer (M) and protofibrils (pf). The unilamellar vesicles were characterized by CryoTEM and Dynamic light scattering and the bilayer thickness is characterized using small angle x-ray scattering. We have investigated the aggregation kinetics of Aβ42 with and without liposomes using Cryo transmission electron microscopy. We have investigated the effect of Aβ42 monomer and protofibrils on the dynamics of unilamellar vesicles using quasielastic neutron scattering. CryoTEM study shows a higher aggregation of amyloid Aβ42 in presence of brain phospholipids and the onset of fibrillation. This study shows Aβ42 brain phospholipids association and the impact of Aβ42 on the dynamics of unilamellar vesicles extracted from brain tissues on the picosecond time scale and Aβ42 fibrillation kinetics.

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Targeted use of residual stress in electrical steel to increase energy efficiency

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Stacked electrical steel sheets compose the magnetic core of electric engines, in which the magnetic flux is guided by cut-outs in the sheets. We developed magnetic flux guidance by targeted residual stress instead of cut-outs to increase the maximum achievable rotational speed of electric engines by increasing the mechanical stability. Due to a combination of limitations, we primarily probed the electrical steel sheets using neutron grating interferometry. To further understand the connection between residual stress and magnetic properties of electrical steel, we would like to discuss additional measurement and simulation techniques, such as strain-mapping, X-ray diffraction or micro-magnetic simulations.

Parallel 5 / 53

A Bayesian approach to fit Molecular Dynamics (MD) simulations to neutron and X-ray diffraction and spectroscopy data on the example of water

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Most of the established MD water models are optimized to reproduce macroscopic water properties, but are then used to study its nanoscopic structure and dynamics.
Neutron and X-ray scattering experiments investigate matter on exactly this nanoscopic level and these experiments can be used to optimize the water models on exactly the same time- and length-scale they will be evaluated on.

In our work, we connect published experimental data of neutron and X-ray experiments on liquid water (diffuse scattering and quasielastic neutron scattering) with MD simulations via a Bayesian fitting algorithm to obtain a set of parameters that can simultaneously fit the real nanoscopic structure and dynamics on an atomic level. To do so, we tie together existing best-of-class tools for MD simulation (LAMMPS) and scattering curve computation (Sassena) using a self-written Bayesian framework that samples the parameter space with a Markov Chain Monte Carlo approach.

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Defect detection in additively manufactured metal components using neutron grating interferometry

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Additive manufacturing (AM) enables to manufacture of complex shapes ultimately leading to lightweight components. To be certain that the components perform as designed it is necessary to know the types of defects and distributions in the components and their influence on mechanical properties. For this neutron grating interferometry (nGI) can be used to quantify various types of defects and to visualise the defect evolution under loading conditions.

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LiBH4 as a liquefying catalyst for hydrogen release/uptake from a storage material

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Hydrogen as energy carrier is one of the hot topics aimed at stopping global warming. Hydrogen storage is one of its challenges. The problems of storage in high-pressure vessels and liquefaction (physical methods) are, firstly, high energy requirements and, secondly, hydrogen leaks through vessel walls via diffusion. When stored chemically, H_2 is produced only on demand. This overcomes the escape threat and, provided there are moderate operation conditions, it is also an energy saving method. Lightweight complex hydrides are ionic compounds which consist of an anion complex, where hydrogen is covalently bonded to a central metal or non-metal atom, and one or several metal cations. They have high gravimetric hydrogen density and are capable of reversibly releasing and up-taking hydrogen. Due to their low weight, they are particularly advantageous for mobile applications. Amides (NH_2^-), are one class of these light-weight complex hydrides. Obstacles preventing their use are high operation temperatures (energy cost) and the release of NH_3 under heating (due to fuel cell poisoning, which requires regeneration afterwards, and quantitative reduction of the desorbed hydrogen gas). However, when amides are mixed with hydrides (e.g. $Mg(NH_2)_2$ with LiH), NH_3 is caught by the latter, leading to hydrogen generation. A $6Mg(NH_2)_2-9LiH$ mixture is in principle a good storage candidate but the kinetics are sluggish and high operation temperatures are required. This is solved when using lithium borohydride $LiBH_4$ as an additive: it plays the role of a catalyst. Lithium amide $LiNH_2$, created in the first step of the hydrogen release reaction, forms a mixture with $LiBH_4$. Two known compounds, $Li_2BH_4NH_2$ (melting at 90℃) and $Li_4BH_4(NH_2)_3$ (melting at 190℃), form an ion-conducting liquid at working conditions. It is assumed that this accelerates the reaction. Varying the quantity of $LiBH_4$ changes the resulting mixture properties by forming different $LiBH_4$–$LiNH_2$ mixed phases. I will present the binary phase diagram ($LiBH_4$–$LiNH_2$), obtained from DSC and diffraction measurements, indicating $LiBH_4 : LiNH_2$ ratios with corresponding $6Mg(NH_2)_2 : 9LiH : xLiBH_4$ compositions. Such juxtaposition is a prerequisite for understanding the reaction mechanisms in these hydrogen storage materials.

Innovative beam monitoring approaches for NEPOMUC.

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The second largest cause of measurement time loss at NEPOMUC is the time spent to optimize the positron beam to the specification required by the user; the speed of this optimization process is primarily determined by the available detection techniques. As modern positron spectroscopy requires beams of ever higher intensity and focus, it is paramount for our complex to develop and adopt faster and more precise diagnostics. I will present here two novel approaches to the detection of the position, shape and intensity of a low-energy positron beam developed by our team.

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

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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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Ongoing Positron Annihilation Doppler-Broadening Spectroscopy at the MLZ

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We are able to perform measurements for defect analysis by using a monoenergetic positron beam for Doppler-broadening spectroscopy.
The positrons are provided by a β^+ radio-isotope and moderated in a 1 µm tungsten mono-crystal.
Recent measurements include defect studies on tungsten mono-crystals, tungsten oxide films, Al alloys, and NV centers.

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SANS-1MAX: Massive Q-Range Upgrade

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The SANS-1MAX proposal aims both at extending the dynamical Q-range and increasing the maximal momentum transfer Q. The SANS-MAX proposal consists of two independent two subprojects. (i) The replacement of the S-bender neutron guide with an optimized version will shift the wavelength cut-off down to ~2.5 Å. (ii) The installation of a second, high-Q detector bank at short detector distances on a second, independent detector carriage will largely improve the dynamic range.

Both upgrades will enable the access to new fields of research, particularly for modern engineering materials science and metallurgy applications and energy materials. The increased dynamical Q-range is particularly beneficial for the growing demand of in-situ measurements of irreversible processes, e.g., precipitation growth in high performance alloys, quenching of alloys, rapid heating and cooling processes and the mimicking of metal process chains, in particular in combination with sample environment like the dilatometer. Accessing larger Q allows measuring even smaller correlations of a few atoms to study the early growth of precipitates. A maximum momentum transfer of 2.2 Å^-1 of the SANS-1MAX proposal will finally allow covering the first Bragg peaks of typical alloys like e.g. Ni or Co based superalloys and their main precipitates. This option will enable coherent investigations of early stage precipitation covering the SANS and diffraction region in a single measurement. It hence allows an analysis of the size, size distribution, shape and the crystalline properties of precipitates. Besides materials science, SANS-1MAX will also tremendously increase the overall efficiency of SANS-1.

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Sodium-22 Based Measurements at the Coincident Doppler-Broadening Spectrometer

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The Coincident Doppler-Broadening Spectrometer (CDBS) at NEPOMUC provides in depth information about open volume defects and their chemical surroundings. While usually operated with the reactor based NEutron induced POsitron source MUniCh (NEPOMUC), the time in between reactor cycles can be used for Sodium-22 based measurements. This means that the sophisticated data acquisition hardware of the CDBS can me utilised more efficiently. This opportunity has been used to perform measurements on structural AlCu alloys. Additionally, high statistics measurements on W and Kapton samples to investigate the positron thermalisation process were performed.

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Status update of ODIN, the neutron instrument for imaging at ESS

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ODIN is the ESS state-of-the-art multipurpose neutron imaging instrument. Using wavelength-resolved imaging with tunable medium to high wavelength resolution, ODIN will provide significantly increased chemical and structural sensitivity compared to other traditional neutron imaging instruments, with fixed (or absent) wavelength resolutions. ODIN will view both the cold and the thermal moderators enhancing its spectral flexibility. Ten choppers, together with the neutron extraction and guide system, are the main instrument components behind ODIN´s flexible performance. Nine choppers are located inside the bunker, together with the heavy shutter, while the remaining frame overlap chopper is in the experimental hall D01. The cave is divided in the beam shaping area, with a variable pinhole and filter systems, and the experimental area with sample stages, flight tubes and detector systems; it will also provide ample space for sample environments, other equipment needed for specific imaging modalities (such as an x-ray source), as well as for future upgrades like a diffraction detector. ODIN is now in its installation phase, after two and a half years of detailed design, procurement and manufacturing of all the components. Here we will present some of the design highlights and how the challenging installation is accomplished in the framework of the ESS facility at Lund, Sweden.

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Current status and future of the NECTAR instrument utilizing thermal and fast neutrons

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Over the past years, NECTAR has received multiple upgrades, including a new translation/rail system, a scintillator changer, scraper for fast neutrons, and event mode imaging capabilities. The upgrades improve existing capabilities but also enable more advanced new techniques, such as multimodal imaging and event-based neutron imaging. Here, we propose to discuss the current status, as well as the future of the NECTAR instrument with new advanced methods for the world wide only instrument that offers fast neutrons at a large scale international user facility.

Parallel 5 / 42

Investigations of cell biology with neutron scattering

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Neutron scattering provides a statistical non-destructive perspective on structure and dynamics in living cells over a range of time and length scales. Simple model systems, red blood cells, and photosynthetic organisms have been examined to understand the nanoscale changes associated with cellular metabolic activity. Here we examine the unique contribution of the neutron perspective to understanding these systems, and the complementarity of the perspective to other experimental techniques.

Parallel 5 / **29**

Discussion about purchasing an X-Ray μ-focus CT for MLZ

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X-rays often provide complementary information to neutrons in imaging and diffraction applications. Modern X-ray microfocus CT machines provide capabilities that are normally only available at synchrotron sources on a lab scale. While the measurement times are obviously longer, spatial resolution in the sub-μm regime as well as modalities such as phase contrast imaging or crystal grain mapping become available with such devices. We will show some of the possible applications of modern x-ray CT machines beyond classical absorption CT with the aim to start a discussion about possible applications to complemenmt the neutron science performed by MLZ employees and users.

Plenary 1 / **71**

Activities of the Data-Driven Discovery Group on Data Reduction for MLZ Instruments

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Plenary 1 / **72**

Oscillatory rheology of (soft) structured materials: insights and future perspectives

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