MLZ USERS2019

Marriott Hotel Munich – December 10th to 11th, 2019

TUESDAY

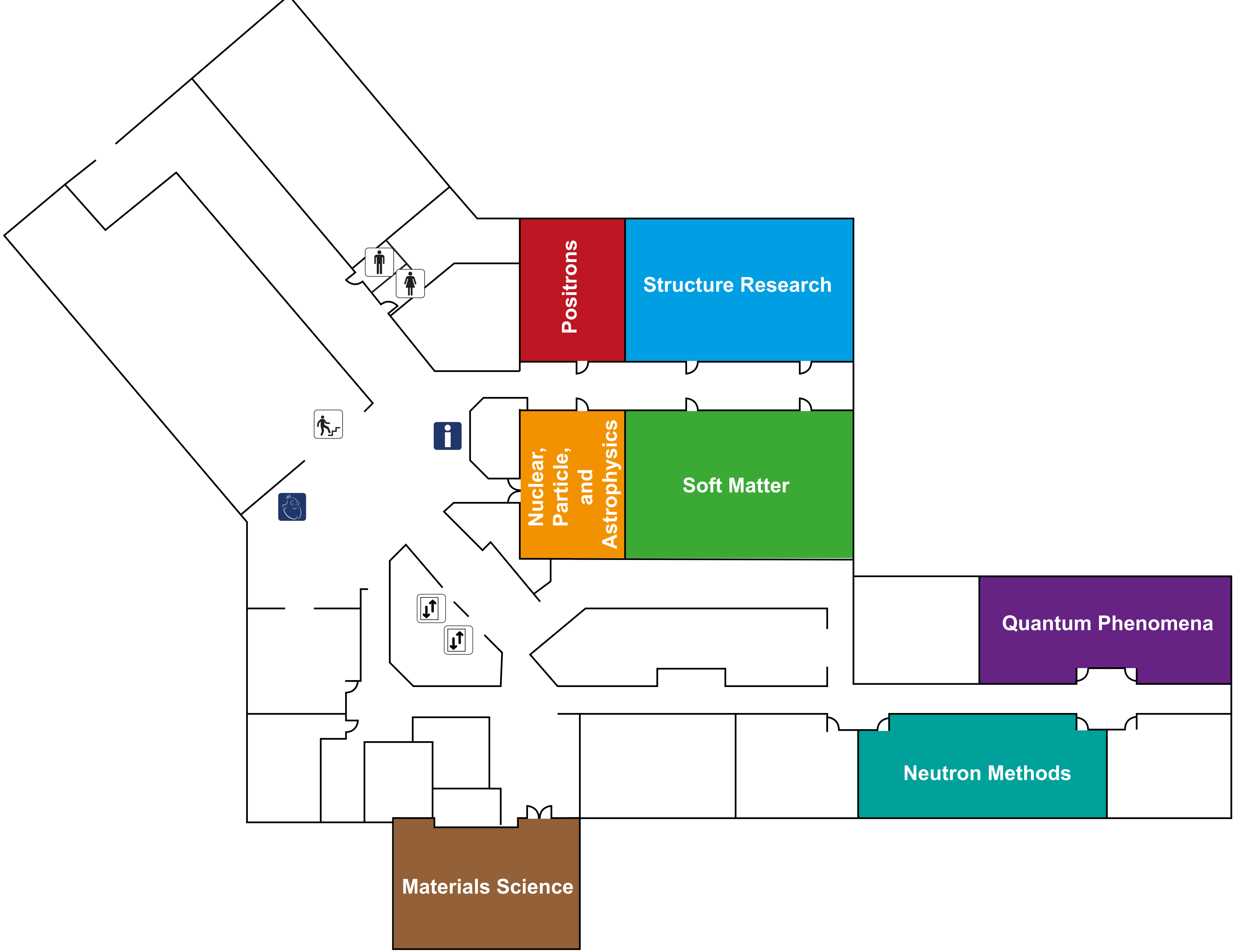
WEDNESDAY

***Instructions**:*
Just click on the name of the day you like to see.
Tables of the day are linked to the sessions.
Tables of sessions are linked to the abstracts.
By clicking on the icon on the top of each page you will go back to this page.

MLZ is a cooperation between:
JÜLICH Forschungszentrum
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung
Technical University of Munich TUM

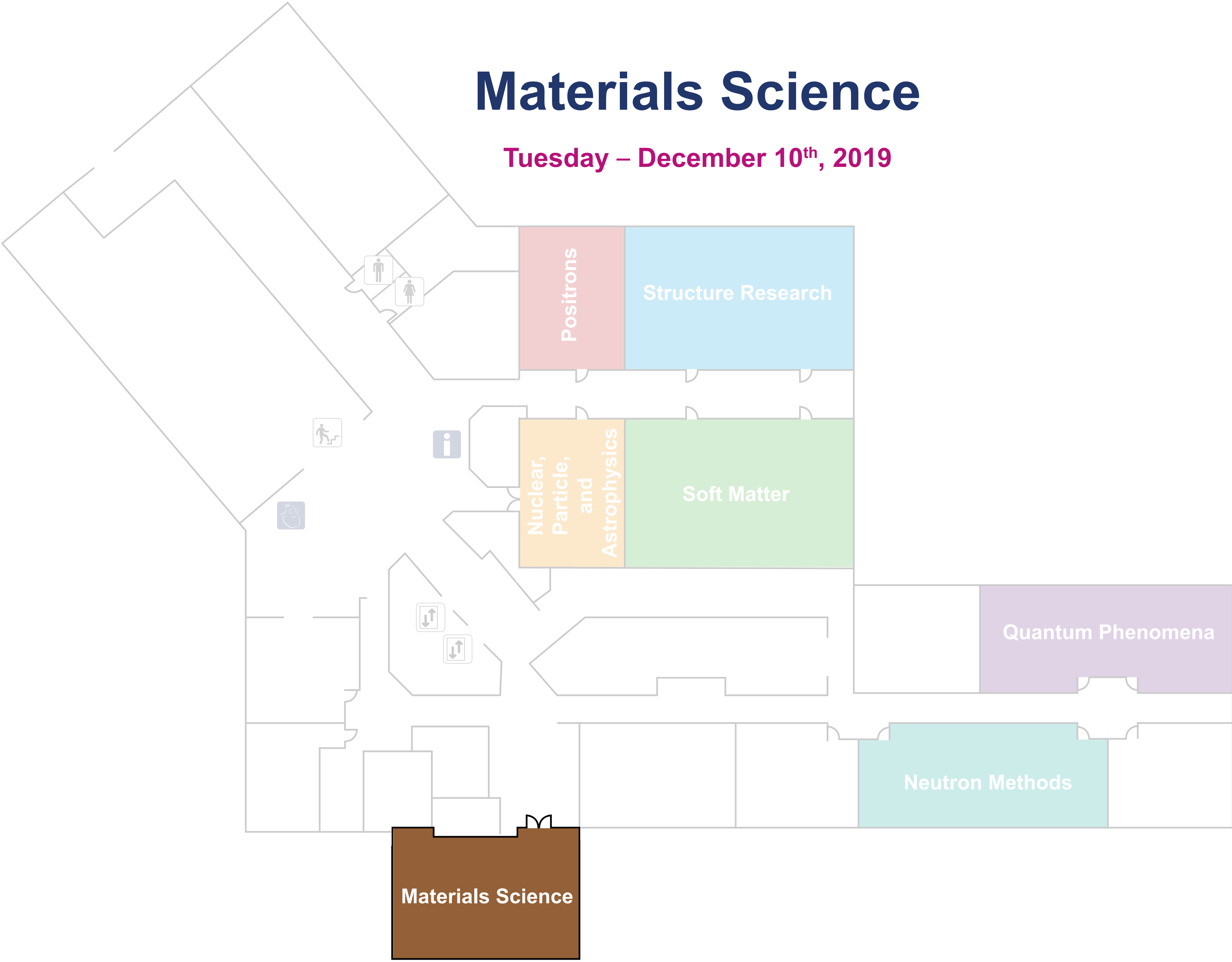
TUESDAY

12:00	Lunch						*Marriott Hotel Munich, Berliner Str. 93, 80805 München*
13:00 - 14:30	Materials Science I	Neutron Methods I	Nuclear, Particle, and Astrophysics I	Quantum Phenomena I	Soft Matter I	Structure Research I	Positrons I
14:30	Coffee break						*Marriott Hotel Munich*
15:00 - 16:30	Material Science II	Neutron Methods II		Quantum Phenomena II	Soft Matter II	Structure Research II	Positrons II
16:30	Coffee break						*Marriott Hotel Munich*
17:00 - 18:00	Materials Science III	Neutron Methods III		Quantum Phenomena III	Soft Matter III	Structure Research III	Positrons III
20:00	Dinner						*Zum Franziskaner, Residenzstr. 9, 80333 München*


Positrons
Structure Research
Nuclear, Particle, and Astrophysics
Soft Matter
Quantum Phenomena
Neutron Methods
Materials Science

Materials Science

Tuesday – December 10th, 2019



click here to go to first page of this workshop

Materials Science I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:27	**Influence of alloying elements on high-temperature structure and microstructure of Co-Re base alloys**	*Pavel Strunz*
13:27 - 13:42	**Ex- and in-situ measurements with dilatometer**	*Martin Landesberger*
13:42 - 13:57	**Magnetic property evaluation in electrical steel at ANTARES**	*Lucas Boehm*
13:57 - 14:12	**Residual stress and FEM modeling in metal matrix composites**	*Xingxing Zhang*
14:12 - 14:27	**Deformation induced martensitic transformation in NiMnGa ferromagnetic shape memory alloys studied by in-situ neutron diffraction**	*Yudong Zhang*

Influence of alloying elements on high-temperature structure and microstructure of Co-Re base alloys

**Pavel Strunz (Nuclear Physics Institute of the AS CR ·
Department of Neutron Physics)**

Tuesday, 13:00

Debashis Mukherji (TU Braunschweig), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Lukas Karge, Přemysl Beran (Nuclear Physics Institute of the CAS), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Joachim Roesler (TU Braunschweig, Institut für Werkstoffe)

Co-Re-based alloys [1] are being developed to supplement single crystal Ni-based superalloys in future gas turbines. Higher operation temperatures are foreseen for them enabling a higher efficiency of energy conversion and thus lower fuel consumption. Alloying elements with various functionality are added to these alloys, for example Re to increase melting temperature, Cr or Ni for oxidation resistance, C and Ta to produce high-temperature strengthening phase (TaC), or boron to improve ductility [2]. We report in situ neutron scattering investigations at elevated temperatures of B, Ta and Ni addition effects on structure and microstructure. First, boron influence [3,4] on stability of the matrix at the foreseen metal operation temperatures (≥1200°C), then optimum ratio of Ta and C for improved strengthening [5], and, finally, influence of Ni on hcp – fcc transformation [6] temperature and sigma phase content [7]. TaC were found to be a suitable high-temperature strengthening phase up to 1200°C. Neutron scattering proved that boron addition is not detrimental for high-temperature stability of the matrix.

[1] J. Rösler et. al, Adv. Eng. Mater. 9, 876–881 (2007)

[2] D. Mukherji et al, Scripta Mat. 66, 60–63 (2012)

[3] P. Strunz et al, Met. Mat. Int. 24, 934-944 (2018)

[4] P. Beran et al, Metals 8, 621 (2018)

[5] L. Karge et al, Acta Mat. 132, 354-366 (2017)

[6] D. Mukherji et al, Met.Mat.Trans.43A, 1834-44 (2012)

[7] P. Beran et al, Adv. Mater. Sci. Eng. 2018, 5410871 (2018)

Ex- and in-situ measurements with dilatometer

**Martin Landesberger (Lehrstuhl für Umformtechnik
und Gießereiwesen utg, Technical University of Munich)**

Tuesday, 13:27

The phase transition kinetics in austempered ductile iron (ADI) and perferritic ductile iron (IDI) are investigated by means of neutron diffraction and dilatometry at the STRESS-SPEC instrument. Measurements with the new TA Instruments 805 A/D quenching dilatometer characterize in-situ the transition from austenite to ferrite. The short instrumental setup description is followed by a comparison of achieved results by dilatometry and neutron diffraction. Both methods give insight into the carbon enrichment at austenitization temperature of 900°C as well as on the subsequent quenching process to isothermal annealing temperature between 300°C and 400°C. The quenching of the material leads to ausferritic microstructure formation during annealing which contains retained austenite, acicular ferrite and graphite nodules. The addition of alloying elements like Cu or Mo leads to a retardation of the decomposition of the retained austenite and opens a process window for heat treatment before carbide formation sets in. The influence of the alloying element Mo on the decomposition of retained austenite is presented. The macroscopic length change evaluated by dilatometry is influenced by phase transition and carbon enrichment of the retained austenite. Neutron diffraction enables distinguishing between the lattice expansion caused by both effects.

Magnetic property evaluation in electrical steel at ANTARES

Lucas Boehm (Lehrstuhl für Umformtechnik und Gießereiwesen utg, Technical University of Munich)

Tuesday, 13:42

Rotors and stators made from electrical steel are core elements of electric machines. Typically, these are built up of thin shear cut lamellae. However, due to the cutting process, residual stress is introduced into the lamellae and it was found that this detrimentally alters the magnetic properties of the material. The magnetic properties of electrical steels are related to their domain structure and residual stress hinders domain growth in electric fields. With the help of Neutron-Grating-Interferometry (NGI) and a magnetizing yoke, the domain wall density in the cutting affected area of shear cut samples can be evaluated at different field strengths. Generally, a high domain wall density indicates poor magnetic properties. This approach allows to compare different cutting strategies with regard to resulting magnetic properties. More than that, Neutron-Grating-Interferometry allows to determine a gradient of magnetic property deterioration from the cutting edge to the inner regions of the sample. The results of the NGI-measurements are in good accordance with FEA calculations and contribute continuously to their improvement. In this research project, different cutting clearances, materials, and tool geometries are investigated at the cold neutron radiography and tomography station (ANTARES) of MLZ with the aim of finding production strategies for loss-optimized electric machines.

Residual stress and FEM modeling in metal matrix composites

Xingxing Zhang (Institute of Metal Research, Chinese Academy of Sciences)

Tuesday, 13:57

Residual stresses (RSes) in metal matrix composites (MMCs) are more complicated than in homogeneous materials. They can be divided into macro and micro (elastic mismatch, thermal misfit and plastic misfit) RSes. Therefore, precise characterization of RSes in MMCs is difficult. Previous method for diffraction-based RS analysis in MMCs has several drawbacks [1-3].

In the past few years, a new and reliable method is developed by the authors for diffraction-based RS analysis in MMCs [4]. By using this method, the macro and micro RSes in friction stir welded SiC/Al composites were determined [4]. The effects of welding parameters and post weld heat treatment were assessed. Furthermore, a multiscale finite element model is developed to predict the RSes [5-7].

[1] Fitzpatrick ME, Hutchings MT, Withers PJ. Acta Mater. 1997;45:4867.

[2] Eshelby JD. Proc R Soc Lon Ser-A 1957;241:376.

[3] Mercier S, Jacques N, Molinari A. Int. J. Solids Struct. 2005;42:1923.

[4] Zhang XX, Ni Dr., Xiao BL, Andrae H, Gan WM, Hofmann M, Ma ZY. Acta Mater. 2015;87:161.

[5] Zhang XX, Xiao BL, Andra H, Ma ZY. Compos. Struct. 2016;137:18.

[6] Zhang XX, Wang D, Xiao BL, Andrae H, Gan WM, Hofmann M, Ma ZY. Mater. Des. 2017;115:364.

[7] Zhang XX, Wu LH, Andrä H, Gan WM, Hofmann M, Wang D, Ni dr, Xiao BL, Ma ZY. J. Mater. Sci. Technol. 2019;35:824.

click here to go to first page of this workshop

Deformation induced martensitic transformation in NiMnGa ferromagnetic shape memory alloys studied by in-situ neutron diffraction

Yudong Zhang (Université de Lorraine, CNRS)

Tuesday, 14:12

Naifu Zou (Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University), Zongbin Li (Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University), Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Xiang Zhao (Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University), Claude Esling (Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3), Liang Zuo (Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University)

For Ni-Mn-Ga ferromagnetic shape memory alloys, the martensitic transformation produces lattice strain. Appling external deformation during the transformation imposes specific constraints to the lattice deformation thus may change the strain path of the phase transformation. To elucidate such changes, we performed in-situ neutron diffraction inspection on the Ni50Mn30Ga20 samples with 7M martensite during their thermo-mechanical treatments. The sample was first fully austenitized and then cooled to allow the occurrence of the martensitic transformation. Then the same thermal cycle was repeated and a compressive load was applied during the isothermal holding and the cooling process. Two stresses of 20 and 50 MPa were used, respectively. The stress-free and the stress-assisted transformations were studied by in-situ neutron diffraction. It is found that under a compressive load of 20 MPa, austenite transforms to 5M martensite instead of the normal 7M martensite generated following the Pitsch OR. When the compressive load was increased (50 MPa), austenite also transforms to 7M martensite but under a new OR in addition to the 5M martensite. The 5M martensite then further transformed to 7M martensite during the subsequent cooling. The formation of the new martensite products following the different transformation paths under the applied compressive load allows a maximum accommodation of the imposed macroscopic deformation by the transformation lattice deformation.

Materials Science II

Tuesday – December 10th, 2019
15:00-16:30

15:00 - 15:27	**Is it stabilized? PGAA as a tool for the determination of desalination success of archaeological iron objects**	*Britta Schmutzler*
15:27 - 15:42	**Morphology investigation of the active layer of hybrid solar cells with GISANS**	*Volker Körstgens*
15:42 - 15:57	**Structure of a deep eutectic solvent at the silicon surface**	*Nebojša Zec*
15:57 - 16:12	**Non-Destructive Bulk Analysis of Critical Metals in Smartphones**	*Jens Walter*
16:12 - 16:27	**Breakdown of the Stokes-Einstein Relation Above the Melting Temperature in Liquid Phase-Change Materials**	*Shuai Wei*

Is it stabilized? PGAA as a tool for the determination of desalination success of archaeological iron objects

Britta Schmutzler (FH Erfurt)

Tuesday, 15:00

Zsolt Revay (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Christian Stieghorst (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Cultural heritage made of iron is easily damaged by post excavation corrosion, caused by chloride ions diffusing into the finds during their burial in the soil. Therefore, the chlorine has to be eliminated by conservation treatment, for example by washing the objects in alkaline solutions.

The research project “Besonderes Eise(r)n bewahren” (funded by DBU) is designed for comparison of varying desalination treatments by quantifying the residual chlorine content after the conservation treatment. So, the less chlorine, the more efficient a treatment was, the safer the object and the archaeological record can be.

PGAA was the chosen method for chlorine measurement since it is non-destructive and therefore allows pre- and post-test-design of the experiments. It was tested in a large scale approach with 33 days measurement time and 128 measurements of totally 120 objects. Despite of changed mounting system during the project’s runtime and heterogeneous sample material, the results were reproducible. Several alkaline solutions turned out as effective and low cost strategy for conserving archaeological iron objects.

Finally, PGAA is a great opportunity to measure the chlorine content of archaeological objects in a non-destructive and precise way, and can be used as a control, if the conservation treatment was successful, and if the cultural heritage could be preserved by treatment.

Morphology investigation of the active layer of hybrid solar cells with GISANS

Volker Körstgens (Department of Physics, Technical University of Munich)

Tuesday, 15:27

Volker Körstgens (Technical University of Munich), Lautaro Diaz Piola, Christina Geiger, Lucas Kreuzer (Technical University of Munich, Chair of Functional Materials, Garching), Tobias Widmann (Technical University of Munich, Physik Department, LS Funktionelle Materialien), Klara Stallhofer, Hristo Iglev, Reinhard Kienberger, Gaetano Mangiapia (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Peter Mueller-Buschbaum (Technical University of Munich, Physik-Department, LS Funktionelle Materialien)

In the development of non-conventional solar cells not only the achievements of highest power conversion efficiencies and maximum lifetime of devices is of interest. Also the sustainability of the production process of the devices comes into focus. Following this idea, we developed hybrid solar cells with an active layer based on low temperature processed titania and a water-soluble polythiophene [1]. In our approach titania nanoparticles are produced with laser ablation in liquid in order to initiate a functionalization of titania with the polymer for the active layer. The devices and the investigated active layers were produced with spray deposition. With the spray deposition technique the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. In order to understand the structure - function relation we investigated the morphology of the spray-deposited active layers with tof-GISANS at the REFSANS instrument at MLZ, Garching.

[1] V. Körstgens et al., Nanoscale 2015, 7, 2900-2904.

click here to go to first page of this workshop

Structure of a deep eutectic solvent at the silicon surface

Nebojša Zec (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Tuesday, 15:42

Gaetano Mangiapia (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Mikhail Zheludkevich (Helmholtz Zentrum Geesthacht (HZG)), Jean-Francois Moulin (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

The main aim of this work is to reveal the structure of the layers formed at the interface between deep eutectic solvents (DES) and silicon surface with and without applied constant electric potential using neutron reflectometry (NR) and molecular dynamics simulations (MDs). Work is focused on finding experimental evidence for an ordered layer of DES over an Si substrate under DC conditions and resolving the destruction of this layer by a superimposed AC field. Electrochemical experiments have shown that application of the potential of -1.6V superimposed with alternating sinusoidal component of 50 mV allows zinc depostion. Increasing temperature has the same effect and at 100 degrees C electrodeposition is possible even in potentiostatic regime. The results obtained with REFSANS instrument at Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich are compared with the reflectivity calculated from molecular dynamics simulations. Through this work we tend to determine the relationship between NR measurements of DES/silicon interface and the corresponding structural information obtained by MD simulations of the same system.

Non-Destructive Bulk Analysis of Critical Metals in Smartphones

Jens Walter (Georg-August Universität Göttingen)

Tuesday, 15:57

Nicole Nolte-Moser (MASA Institute), Klaus Wemmer (Georg-August Universität Göttingen), Sebastian Merk (Georg-August- Universität Göttingen), Zsolt Revay (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Commonly, smartphones contain about 30 different metals [1]. From these many are considered as Critical Raw Materials (CRMs), as they are economically very important combined with high supply risks and a lack of viable substitutes [2,3]. Therefore, they are critical for a sustainable economy [3]. Additionally, most of these elements are mined under devastating social and/or ecological conditions and are often subject to unfair trade [4]. Especially, the strongly versatile and growing smartphone market has a high demand on many of these partly highly critical metals. However, hardly any scientific data is available about the market consumption of these critical metals, which is essential to develop technical and economic concepts to overcome existing critical aspects.

These new concepts are strongly developed by some smartphone manufacturers, especially to compensate negative ecological and social effects from mining and trade of these metals. Their aim is to provide the market with sustainable smartphones. To gain insight, 3 different mobile phones were analysed by PGAA and NAA. This study was performed to test firstly the suitability of these methods and secondly to compare metal compostions of different smartphone manufacturers, one of them developing sustainable smartphones. We present first results.

References:

[1] www.informationszentrum-mobilfunk.de/umwelt

[2] ec.europa.eu/growth/sectors/raw-materials/

[3] criticalrawmaterials.org

[4] www.amnesty.org/en/latest/news/

Breakdown of the Stokes-Einstein Relation Above the Melting Temperature in Liquid Phase-Change Materials

Shuai Wei (RWTH Aachen)

Tuesday, 16:12

The dynamic properties of liquid phase-change materials (PCMs), such as viscosity η and atomic self-diffusion coefficients D, play an essential role in ultrafast phase switching behavior of novel non-volatile phase-change memory applications. To connect η to D, the Stokes-Einstein relation (SER) is commonly assumed to be valid at high temperatures near or above the melting temperature T_m and is often employed for assessing liquid fragility (or crystal growth velocity) of technologically important PCMs. However, using quasi-elastic neutron scattering (QENS), we provide experimental evidence for a breakdown of the SER even at temperatures above T_m in the high-atomic-mobility state of well-known PCMs $Ge_1Sb_2Te_4$, $Ge_2Sb_2Te_5$, $Ag_4In_3Sb_{67}Te_{26}$(AIST), and GeTe. This implies that although the viscosity may have strongly increased during cooling, the diffusivity can remain high due to the early decoupling, being a favorable for fast phase switching behavior of the high-fluidity PCM. We discuss the origin of the observation and propose the possible connection to a metal-semiconductor and fragile-strong transition hidden below T_m. In addition, the infinite-frequency shear modulus is experimentally determined ranging from 2 to 3GPa for liquid PCMs, which permits extracting viscosity from microscopic structural relaxations usually accessible to simulations and scattering techniques.

click here to go to first page of this workshop

Materials Science III

Tuesday – December 10th, 2019
17:00-18:00

17:00 - 17:15	**Charging and Aging Mechanisms of Si/C Composite Anodes – An Operando Neutron Scattering Study** *Thomas Waldmann*
17:15 - 17:30	**Neutron radiography for visualization of the filling process in the production of lithium ion cells** *Florian Günter*
17:30 - 17:45	**Multiprobe Imaging using Neutrons and Gammas at the NECTAR Beam-Line** *Adrian Losko*
17:45 - 18:00	**SEI growth influences at Li-Ion cells caused by formation, cycling and lamination revealed using NDP** *Martin Frankenberger*

Charging and Aging Mechanisms of Si/C Composite Anodes – An Operando Neutron Scattering Study

Thomas Waldmann (ZSW – Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg)

Tuesday, 17:00

Karsten Richter (ZSW – Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg), Neelima Paul (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Jobst Nicola (ZSW – Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg), Rares George Scurtu (ZSW – Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Margret Wohlfahrt-Mehrens (ZSW – Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg)

Interesting candidates to fulfill the requirement of higher specific energy in Li-ion batteries are Si/C composite anodes. We investigated the charging mechanisms in commercial 18650 cells (anode: graphite + 3% Si, cathode: NCA)[1] via operando neutron diffraction with the STRESS-SPEC instrument at the neutron source FRM II in Garching.

Although the amorphous Si compound did not allow following the Si alloying directly, it can indirectly be observed by the relaxation of the LiC_6 and LiC_{12} reflexes, similar like for Li deposition.[2] Charging at 0.1C, 0.5C, and 0.75C showed different mechanisms. Interestingly, we find a transfer of Li from graphite into the Si compound which was, to best of our knowledge, not reported before. The measurements are complemented with simultaneous electrochemical measurements and Post-Mortem analysis (SEM and GD-OES depth profiling [1]) after cell disassembly. The unique capabilities of the used methods, especially operando neutron diffraction at FRM II give very interesting novel insights into battery materials, which will allow improvement of later battery generations.

[1] K. Richter et al., J. Electrochem. Soc. 165 (2018) A3602.

[2] V. Zinth et al., J. Power Sources 271 (2014) 152.

This work is based upon experiments performed at the STRESS-SPEC instrument operated by FRM II at the Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Garching, Germany.

Neutron radiography for visualization of the filling process in the production of lithium ion cells

Florian Günter (Department of Mechanical Engineering, Technical University of Munich)

Tuesday, 17:15

Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Neutron radiography was used in several measurement series at the ANTARES instrument of the FRM II to characterize influences on the filling process in lithium ion cell production. The filling of the cells with electrolyte liquid consisting of iterative dosing and wetting steps is very time-consuming and has a high influence on the cost and quality of the cells. Since it is otherwise not possible to look into the cell during the process, a mobile filling station was built so that the process could be measured in-situ and in-operando. Then the method was used to characterize parameter, electrode design and format influences and thus to optimize the process.

In the talk, the plant design, the measuring method and the results will be presented.

Multiprobe Imaging using Neutrons and Gammas at the NECTAR Beam-Line

Adrian Losko (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Tuesday, 17:30

Dominik Bausenwein (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Thomas Bücherl (Technical University of Munich), Zeljko Ilic, Burkhard Schillinger (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Rudolf Schuetz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

NECTAR is a superior 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 produced in the process. The production of these gamma rays is inevitable as they are inherent with the principles of collimating or stopping the neutrons. 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. Initial results were produced from data measured in the 2019 run-cycle, performed at and supported by the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II). Furthermore, future improvements and advancements for the development of this technique will be discussed.

SEI growth influences at Li-Ion cells caused by formation, cycling and lamination revealed using NDP

Martin Frankenberger (University of Applied Sciences Landshut)

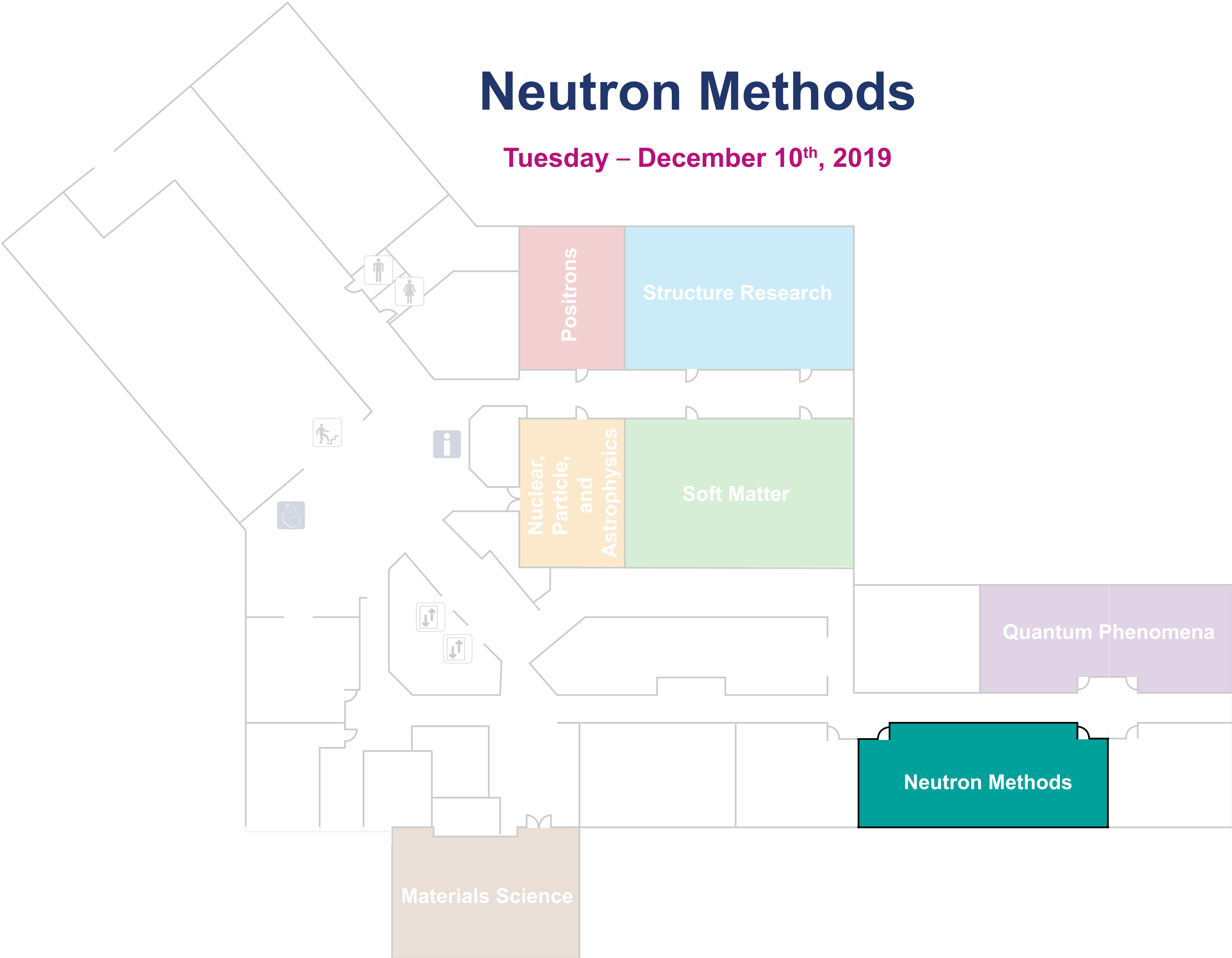
Tuesday, 17:45

Markus Trunk (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Stefan Seidlmayer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Karl-Heinz Pettinger (University of Applied Sciences Landshut)

In this study the influence of an established electrode-separator lamination technique on the formation of solid-electrolyte-interface (SEI) in graphite anodes is investigated. As we have shown previously, the lamination technique is beneficial for the capacity aging in graphite/ $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC) cells. Here, the non-destructive and highly lithium-sensitive Neutron Depth Profiling method (NDP) is used to quantify directly accumulations of lithium in the SEI. Due to the high collimated neutron flux of 3×10^9 $ncm^{-2}s^{-1}$ even traces of lithium can be detected as a function of depth. The anodes were extracted from the graphite/NMC cells, washed and subsequently examined post mortem in fully discharged state. The impact of the charge-discharge cyclying speed as well as the lamination process on the SEI formation was studied via comparing lithium accumulation in laminated and non-laminated anodes at several accelerated formation (0.1C, 1C, 2C) and cycling rates (1C, 2C). Here NDP reveals homogeneous lithium accumulations as function of depth with lithium situated at the surface of the graphite particles thus forming the SEI. The SEI was found to grow logarithmically with cycle number starting with the main formation in the first two cycles. Furthermore, the measurements indicate that the lamination technique hampers the formation of SEI within the anodes in the first charge/discharge cycles..

Neutron Methods

Tuesday – December 10th, 2019



click here to go to first page of this workshop

Neutron Methods I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:45	**Next generation horizontal SANS magnet (NHSM) for quantum phenomena in nanostructures and correlated electron systems** *Sebastian Muehlbauer, Juergen Peters*
13:45 - 14:05	**Modulation of intensity with zero effort - a neutron spin echo technique** *Johanna K. Jochum*
14:05 - 14:30	**The N4DP instrument** *Lukas Werner*

Next generation horizontal SANS magnet (NHSM) for quantum phenomena in nanostructures and correlated electron systems

Sebastian Muehlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)
Juergen Peters (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Tuesday, 13:00

Artem Feoktystov (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

The results of two research studies on the development of the “Next generation horizontal SANS magnet (NHSM) for quantum phenomena in nanostructures and correlated electron systems” are presented. The NHSM project is a high performance compensated 12T horizontal magnet optimized for small angle neutron scattering (SANS), reflectometry and the resonance spin echo technique MIEZE (Modulation of IntEnsity with Zero Effort). The magnet is dedicated for research on quantum phenomena in nanostructures, strongly correlated electron systems and superconductivity.

NHSM will be optimized for lowest possible parasitic background scattering with the least possible amount of material in the beam. Together with a dedicated integrated cryostat, it will offer a wide temperature range of 50mK to 350K. Only the use of modern high-temperature superconducting (HTS) technology will allow the fringe field compensation of a split coil magnet as large as NHSM at reasonable weight (~500kg) and size (75cm x 75cm) enabling the use on a large number of beamlines at MLZ with minimized interference and stray fields. NHSM will be a pioneering project using HTS technology without cryogenic liquids (dry system). As such, NHSM will be the prototype for all future high performance sample environment magnets at large scale neutron scattering or photon scattering facilities.

Modulation of intensity with zero effort - a neutron spin echo technique

Johanna K. Jochum (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Tuesday, 13:45

Christian Franz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Olaf Soltwedel (Physik Department, Technische Universität Darmstadt), Franz X. Haslbeck (Department of Physics, Technical University of Munich), Steffen Säubert (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Andreas Wendl (Department of Physics, Technical University of Munich), Christian Pfleiderer (Department of Physics, Technical University of Munich)

Conventional neutron spin echo (NSE) is an ultra - high energy resolution technique, offering energy resolutions down to <1 neV [1]. However, classical NSE is limited in the range of high energy transfers, reaching an energy resolution of 0.2 meV at best.
Longitudinal neutron resonant spin echo (LNRSE) and longitudinal modulation of intensity with zero effort (LMIEZE) are able to overcome this limitation of classical NSE and NRSE by means of the effective field subtraction method [2]. In NRSE the solenoids of the classical NSE setup are replaced by a pair of resonant spin flippers.
MIEZE is a NRSE technique, that is insensitive to depolarising (e.g. magnetic) samples, as well as depolarising sample environments, such as magnetic fields. Furthermore, MIEZE does not produce the 2/3 background arising from incoherent scattering that is present for classical NSE and NRSE and is therefore well suited for hydrogen containing or other incoherently scattering samples.
In essence, MIEZE is a high-resolution, spin-echo, time-of-flight (TOF) technique where all beam preparation is performed in front of the sample. Typical applications for MIEZE are the investigation of quantum phase transitions, superconductors, vortex lattices, skyrmions, ferromagnetic materials and hydrogen containing samples [3].

[1] B. Farago et al., Neutron News 26 (3) (2015) 15

[2] M. Krautloher et al., Rev. Sci. Instrum. 87 (12) (2016) 125110

[3] C. Franz et al., J. Phys. Soc. Jpn. 88 (8) (2019) 081002

The N4DP instrument

Lukas Werner (Department of Physics, Technical University of Munich)

Tuesday, 14:05

Markus Trunk (Department of Physics, Technical University of Munich), Roman Gernhäuser (Department of Physics, Technical University of Munich), Bastian Märkisch (Department of Physics, Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Neutron depth profiling (NDP) is a non-destructive nuclear analytical technique. It uses charged particles produced in neutron capture reactions for material analysis. This is done by measuring the energy loss of these particles in a sample and determining the production depth through this energy loss. Thereby a depth profile can be measured.

The N4DP instrument is a new experimental setup at the MLZs NL4b neutron guide. It extends the capabilities of the existing PGAA instrument. This contribution will present the instrument, its current capabilities alongside some selected measurement examples and the upgrades that are planned or going on for this instrument.

click here to go to first page of this workshop

Neutron Methods II

Tuesday – December 10th, 2019
15:00-16:30

15:00 - 15:45	**Neutron scattering in high magnetic fields using HFM/EXED facility at HZB** *Oleksandr Prokhnenko*
15:45 - 16:30	**Spin dynamics in strongly-correlated spin systems: physics and methodology** *Sergei Zvyagin*

Neutron scattering in high magnetic fields using HFM/EXED facility at HZB

Oleksandr Prokhnenko (Helmholtz-Zentrum Berlin)

Tuesday, 15:00

The application of high magnetic fields is a powerful method for revealing the complex behavior in modern materials. In combination with microscopic probe such as neutrons it provides a direct access to static and dynamic correlations in matter. Helmholtz-Zentrum Berlin (HZB) hosts a unique high field facility for neutron scattering. The facility combines neutron scattering with continuous magnetic fields as high as 26 T and temperatures down to 0.1 K. Magnetic field is generated by means of horizontal solenoid High Field Magnet (HFM). The magnet utilizes hybrid technology and reaches 26 T at full power of 4 MW. The tapered inner coil allows neutron-scattering to detectors up to ±15° off the beam axis. Neutron scattering in high fields is performed using the dedicated multi-purpose Extreme Environment Diffractometer (EXED). EXED uses time-of-flight (TOF) polychromatic technique. Combined with 15° magnet rotation it provides a gapless coverage of Q-range from 0.1 up to 12 $Å^{-1}$ for diffraction experiments. The low-Q range can be extended beyond 10^{-2} $Å^{-1}$ using a pin-hole TOF Small Angle Scattering mode. A direct TOF spectrometer mode enables inelastic neutron scattering experiments over a limited Q-range < 1.8 $Å^{-1}$ with an energy resolution of a few percent and incident energies below 25 meV. I this talk I will give an overview of the HFM/EXED facility with main focus on science which has been done using it in the last years.

Spin dynamics in strongly-correlated spin systems: physics and methodology

Sergei Zvyagin (Helmholtz-Zentrum Dresden-Rossendorf)

Tuesday, 15:45

Inelastic neutron scattering (INS) and electron spin resonance (ESR) are two of key spectroscopy techniques, complementing each other and widely employed to study the spin dynamics in strongly correlated electron systems. While ESR is limited to magnetic excitations at Gamma-point, INS can nominally probe the spin dynamics within the whole Brillouin zone. On the other hand, the challenges regarding the sample size and hydrogen content, as well as magnetic-field limitation are not so critical in case of ESR. In this talk I will focus on our recent high-field ESR investigations of some quantum low-dimensional spin systems, supporting a number of INS observations and demonstrating the strength of neutron methods, including the discussion on sample environment issues.

click here to go to first page of this workshop

Neutron Methods III

Tuesday – December 10th, 2019
17:00-18:00

17:00 - 17:20	**The new high-resolution J-NSE "PHOENIX" at MLZ** *Olaf Holderer*
17:20 - 18:00	**Electronic spectroscopy of quantum materials in high magnetic fields – A proposal for an inter-facility Priority Action in the frame of LENS** *Marc Janoschek*

The new high-resolution J-NSE "PHOENIX" at MLZ

Olaf Holderer (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Tuesday, 17:00

Stefano Pasini (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Tadeusz Kozielewski (Jülich Centre for Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH), Michael Monkenbusch (Jülich Centre for Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH)

Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. In 2017 the Jülich neutron spin echo at MLZ went through a refurbishment of the secondary spectrometer: The old normal conducting main-precession coils have been replaced by a new set of fringe-field compensated, superconducting magnets that were realized following the results obtained for the design of ESSENSE, the proposed high-resolution NSE spectrometer at the ESS. 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, as the first experiments could already confirm. The new configuration yields an improved resolution that 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 new 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 after the refurbishment and some selected examples from the realm of soft matter dynamics that largely rely on the enhanced properties of the new J-NSE.

Electronic spectroscopy of quantum materials in high magnetic fields – A proposal for an inter-facility Priority Action in the frame of LENS

Marc Janoschek (Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institut (PSI))

Tuesday, 17:20

Martin Boehm (Institut Laue-Langevin (ILL)) Eddy Lelièvre-Berna (Institut Laue-Langevin (ILL)), Marek Bartkowiak (Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institut (PSI)), Uwe Filges (Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institut (PSI)), Oliver Kirstein (European Spallation Source (ESS)), Robert Bewley (ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory),Jörg Voigt (Jülich Centre for Neutron Science (JCNS-1) and Peter Grünberg Institut (PGI-4), Forschungszentrum Jülich GmbH), Peter Link (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Oleg Kirichek (ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory), Marko Marton (Department of Neutron Spectroscopy, Research Institute for Solid State Physics and Optics), Jürgen Peters (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Alexander Holmes (European Spallation Source (ESS)), Alexander Weber (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Peter Willendrup (Department of Physics, Technical University of Denmark, Denmark)

Neutron spectroscopy is a powerful tool to study magnetic excitations arising from correlation effects of electrons. Less well known is that neutrons can also be used to investigate directly electronic band structures in strongly correlated metallic quantum matter [1]. Neutrons scatter electrons form occupied to unoccupied states with a probability given by the so-called Lindhard susceptibility. Although weak in nature, the recent progress in neutron optics on different spectrometers makes now such kind of spectroscopy accessible, as demonstrated e.g. on the strongly correlated metals URu_2Si_2 and Pu [2]. Compared to ARPES, electronic neutron spectroscopy has the advantage of enhanced energetic resolution and can be combined with high magnetic fields.

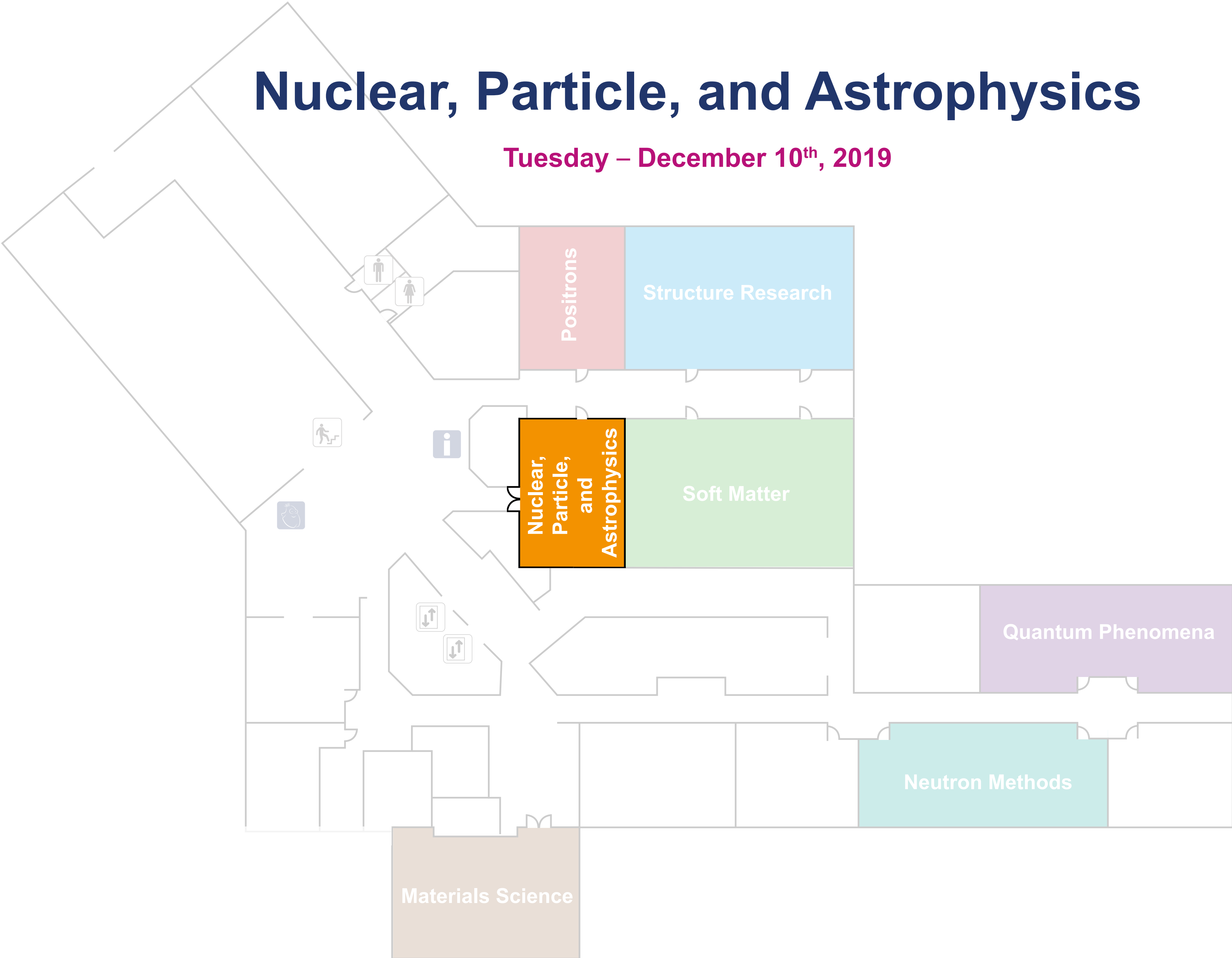
In the frame of the recent inter neutron facility initiative LENS, The League of Advanced European Neutron Sources, we propose to combine electronic spectroscopy with up-to-date unreached continuous magnetic fields on neutron spectrometers, based on all superconducting coils with split-coil geometry. For best signal-to-noise special focusing optics will be included into the magnetic design, optimized with latest Monte Carlo ray-tracing tools combined with finite element calculations. This project is planned as one out of several Priority Actions of LENS, aiming to push the neutron science in Europe to highest standards.

[1] J. F. Cooke et al., Phys Rev B 26, 4410 (1982).

[2] M. Janoschek et al., Sci Adv 1, e1500188 (2015).

Nuclear, Particle, and Astrophysics

Tuesday – December 10th, 2019



click here to go to first page of this workshop

Nuclear, Particle, and Astrophysics I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:30	**Neutron Beta Decay**	*Hartmut Abele*
13:30 - 14:00	**The source for ultracold neutrons (UCN source) at the FRM II**	*Andreas Frei*
14:00 - 14:30	**Status of the neutron decay facility PERC**	*Bastian Märkisch*

Afterwards: Physics Programme at PERC – Collaboration Meeting

Neutron Beta Decay

Hartmut Abele (Vienna University of Technology)

Tuesday, 13:00

We will present new perspectives on neutron beta decay measurements at FRM II.

The source for ultracold neutrons (UCN source) at the FRM II

Andreas Frei (Department of Physics, Technical University of Munich)

Tuesday, 13:30

Werner Adler (Department of Physics, Technical University of Munich), Christian Bocquet (Department of Physics, Technical University of Munich), Stephan Paul (Department of Physics, Technical University of Munich), Johann Schilcher (Department of Physics, Technical University of Munich)

Precision experiments with UCN, such as the search for a possible electric dipole moment (EDM) of the neutron or the measurement of the lifetime of the free neutron, require high UCN densities. Stronger UCN sources are presently developed worldwide, based on the principle of superthermal UCN production, using cryo-converters made of solid deuterium (sD_2) or superfluid helium. At the FRM II a UCN source with a sD_2 converter and sH_2 pre-moderator, placed in a distance of ~60 cm from the central fuel element inside the horizontal, through going beam tube SR6, is currently under construction.

The UCN source has started its non-nuclear test phase. In these tests all parameters how to operate the cooling machines and all necessary auxiliary systems will be varied and optimized in order to freeze out deuterium and hydrogen in a dedicated way, with the simulated nuclear heat load of the FRM II. After the tests, which shall be finished until end of 2018, the whole cooling machine will be transferred to the FRM II, and all the other parts of the source and auxiliary systems will be built and installed.

This talk gives an overview of the current status of the UCN source project at the FRM II.

Status of the neutron decay facility PERC

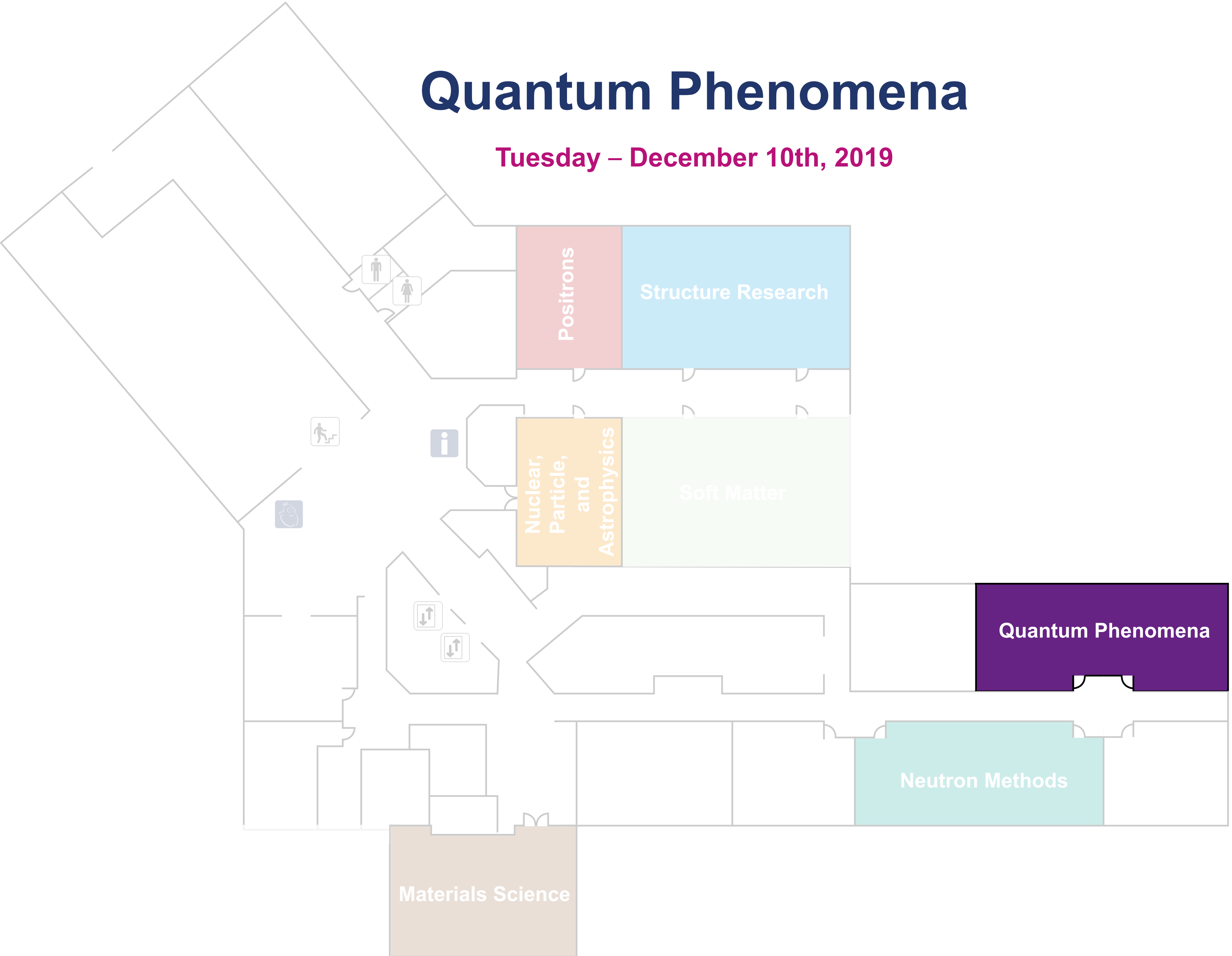
Bastian Märkisch (Department of Physics, Technical University of Munich)

Tuesday, 14:00

Searches for physics beyond the standard model of particle physics are performed at high and at low energies. With the high measurement precision and reliable theory predictions, neutron beta decay experiments address new physics at the 10 TeV scale. We present the status of the upcoming neutron decay facility PERC at the MLZ and discuss future measurements.

Quantum Phenomena

Tuesday – December 10th, 2019



Quantum Phenomena I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:30	**Unique Neutrons: the method for magnetoelastic effects** *Petr Čermák*
13:30 - 14:00	**Topological magnons in frustrated quantum magnets** *Paul McClarty*
14:00 - 14:15	**Single-crystal growth and neutron scattering studies of Mn_3Sn** *Xiao Wang*
14:15 - 14:30	**Interplay of Electronic and Spin Degrees in Ferromagnetic $SrRuO_3$: Anomalous Softening of the Magnon Gap and Stiffness** *Kevin Jenni*

Unique Neutrons: the method for magnetoelastic effects

Petr Čermák (Charles University)

Tuesday, 13:00

Modern condensed matter physics theories are using several assumptions, allowing to solve quantum mechanical problems otherwise hardly solvable. One of them is Born-Oppenheimer approximation: "we can separate motion of nuclei and motion of electrons". It is known for decades that there exist materials with strong magnetoelastic (ME) coupling, where approximation is no longer valid. However, these were treated as exceptional cases until recently. Our pioneering research on intermetallic heavy fermion $CeAuAl_3$ pointed out, that ME coupling is far more common than previously believed and even for weakly ME coupled materials hidden modes influencing its ground state can be present. One of the reasons why this effect was not discovered before is its difficult detection. If you want to measure some effect, your probe must have comparable mass/energy with studied phenomena. It is extremely challenging to directly see crosstalk between electrons and lattice vibrations (phonons) because nuclei are thousand times heavier than electrons. Neutron scattering is probably the only suitable method, thanks to neutron mass and spin.
Consequence: Modern synchrotron sources can substitute neutron measurements in many ways, but observation of electron-phonon coupling will probably never be possible with X-Rays. We should keep it in mind and advertise neutrons correspondingly. Come to the talk and learn more!

Topological magnons in frustrated quantum magnets

Paul McClarty (Max-Planck-Institute (MPI) for the Physics of Complex Systems)

Tuesday, 13:30

I present an overview of recent research into topological magnons in frustrated quantum magnets. By way of illustration, I discuss the case of triplon excitations in the Shastry-Sutherland magnet $SrCu_2(BO_3)_2$. We provide a detailed inelastic neutron scattering data showing the bulk triplon spectrum and its evolution in small magnetic fields. A theoretical analysis of these data based on an interacting hard-core boson model characterizes the main anisotropies in this system and reveals the importance of triplon interactions. We highlight the Berry curvature and triplon band topology in this quantum magnet and discuss future perspectives on this and other systems.I.

Single-crystal growth and neutron scattering studies of Mn_3Sn

Xiao Wang (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Tuesday, 14:00

Yixi Su (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Fengfeng Zhu (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Junda Song (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Thomas Brückel (Jülich Centre for Neutron Science and Peter Grünberg Institut PGI (JCNS-1 / PGI-4), Forschungszentrum Jülich GmbH)

The study of topological quantum materials is among the most active and fruitful fields in condensed matter physics, largely owing to the topologically protected exotic states and emergent phenomena discovered for instance in topological insulators, Dirac and Weyl fermion semimetals. Recent experimental realizations of large anomalous Hall effect (AHE) at room temperature and possible magnetic Weyl fermions in the non-collinear antiferromagnet (AFM) Mn_3Sn, have attracted strong interests on this compound due to its potential applications in antiferromagnetic spintronics and thermoelectric devices. We have prepared high quality Mn_3Sn single crystals via molten flux method and studied its magnetic phase transitions by magnetometer measurement and neutron scattering. Our polarized neutron scattering results show the inverse antiferromagnetic structure at room temperature transferred to modulation phases ambiguously. Besides, the phase dependence of anomalous Hall effect was also confirmed explicitly in our flux grown high quality crystals. This may pave way for the future application in temperature controlling of anomalous Hall effect in spintronics.

Interplay of Electronic and Spin Degrees in Ferromagnetic $SrRu_3$: Anomalous Softening of the Magnon Gap and Stiffness

Kevin Jenni (University of Cologne)

Tuesday, 14:15

Stefan Kunkemöller (University of Cologne), Daniel Brüning (University of Cologne), Thomas Lorenz (University of Colgne), Yvan Sidis (Laboratoire Léon Brillouin (LLB)), Astrid Schneidewind (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Agung A. Nugroho (Institut Teknologi Bandung), Achim Rosch (University of Cologne), Daniel I. Khomskii (University of Cologne), Markus Braden (University of Cologne)

$SrRuO_3$ is one of the very few perovskite metallic ferromagnets; it exhibits anomalous transport, an invar effect, non-Fermi liquid behavior, a magnetic shape-memory effect and it is an important substrate for various oxide heterostructures. Strong spin-orbit coupling (SOC) is visible in the invar effect and the large magnetic anisotropy. Recently, we could grow large single crystals of $SrRuO_3$ using the floating-zone technique [1,2]. We report the first inelastic neutron scattering study of the spin dynamics on single crystals. Our results yield the expected quadratic spin wave dispersion of a ferromagnet. However the magnon gap and stiffness considerably deviate from an earlier inelastic neutron scattering study on powders [3]. In addition we find a non-monotonous temperature dependence of the anisotropy gap and a softening of the magnon stiffness upon cooling. These phenomena can be explained by Weyl physics. We discuss how Weyl modes caused by SOC in $SrRuO_3$ couple electronic and spin degrees of freedom and how this interplay leads to the characteristic behavior in the spin dynamics [4].

[1] S. Kunkemöller et al., Chrys. Res Tec. 51, 299 (2016)

[2] S. Kunkemöller et al., PRB 96, 220406(R) (2017)

[3] S. Itoh et al., Nat. Commun. 7, 11788 (2016)

[4] K. Jenni et al., Phys. Rev. Lett. 123, 017202 (2019)

Quantum Phenomena II

Tuesday – December 10th, 2019
15:00-16:30

15:00 - 15:30	**Orbital selective superconductivity in iron-based superconductors** *Pengcheng Dai*
15:30 - 16:00	**The impact of sample geometry on vortex structures arising in superconductors and chiral magnets - A neutron imaging approach** *Tommy Reimann*
16:00 - 16:15	**Field-angle resolved magnetic excitations in the heavy-fermion metal CeB_6** *Pavlo Portnichenko*
16:15 - 16:30	**Critical dynamics in Ca_2RuO_4 studied by neutron resonant spin-echo spectroscopy** *Matthias Hepting*

Orbital selective superconductivity in iron-based superconductors

Pengcheng Dai (Rice University)

Tuesday, 15:00

Superconductivity in iron-based superconductors emerges from long-range ordered antiferromagnetic phase with nematic order that breaks four-fold rotational symmetry of the underlying lattice. In spite of considerable work over the past decade, much is unclear concerning the microscopic origin of superconductivity and its relationship with magnetism, nematicity, and orbital order. In this talk, I will summarize our recent inelastic neutron scattering studies of iron-based superconductors, focusing on studying the relationship between magnetism, nematic order, and superconductivity. We find that orbital selective magnetic excitations and superconductivity are central to a microscopic understanding of these materials.

The impact of sample geometry on vortex structures arising in superconductors and chiral magnets - A neutron imaging approach

Tommy Reimann (Helmholtz-Zentrum Dresden-Rossendorf)

Tuesday, 15:30

Magnetic flux lines in type-II superconductors as well as skyrmions, are topologically stabilized objects exhibiting strong particle-like behavior. In both cases, the interplay of (i) vortex-vortex interactions, (ii) interactions with the underlying electronic structure and (iii) interactions with impurities results in complex phase diagrams and metastable states. Since the vortices tend to form regular patterns on the sub-µm range, small-angle neutron scattering (SANS) is frequently employed in order to study their nucleation, stability and crystallography. During data evaluation, the sample shape is commonly considered by scaling the applied field according to the sample's demagnetization factor. Since demagnetizing fields are inhomogeneous for non-ellipsoidal cross-section and e.g. corners can act as preferred nucleation sites of vortices, the morphology of the vortex phase may deviates throughout the sample. We demonstrate on the skyrmion lattice in MnSi [1] and the flux line lattice in Niobium [2] that neglecting geometric effects can promote drastic misinterpretation of neutron scattering data. Using complementary neutron radiographic techniques like grating interferometry or diffractive imaging, which provide spatially resolved information about the distribution and morphology of vortex structures, intrinsic effects can be clearly distinguished from geometry induced behavior.

[1] T. Reimann et al., Phys. Rev. B 97, 020406(R)

[2] T. Reimann et al., Nat. Commun. 6:8813

click here to go to first page of this workshop

Field-angle resolved magnetic excitations in the heavy-fermion metal CeB_6

Pavlo Portnichenko (Technische Universität Dresden)

Tuesday, 16:00

Alireza Akbari (Asia Pacific Center for Theoretical Physics (APCTP), Korea), Stanislav Nikitin (Max-Planck-Institute for Chemical Physics of Solids), N. Yu. Shitsevalova (IMPS, Kiev, Ukraine), Petr Čermák (Charles University), Igor Radelytskyi (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Astrid Schneidewind (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Z. Hüsges (Helmholtz-Zentrum Berlin (HZB)), Jianhui Xu (Helmholtz-Zentrum Berlin (HZB)), A. Ivanov (Institut Laue-Langevin (ILL)), J.-M. Mignot (Laboratoire Léon Brillouin (LLB)), Peter Thalmeier (Max-Planck-Institute for Chemical Physics of Solids), Dmytro S. Inosov (TU Dresden)

Hidden-order phases that occur in a number of correlated f-electron systems are among the most elusive states of electronic matter. Their investigations are hindered by the insensitivity of standard physical probes, such as neutron diffraction, to the order parameter that is usually associated with higher-order multipoles of the f-orbitals. The most well-studied member of this family of compounds is the pure CeB_6 material, which is considered a textbook example of a system with the magnetically hidden order, typically associated with an antiferromagnetic arrangement of magnetic quadrupole moments. As a simple-cubic system with only one f-electron per cerium ion, CeB_6 is of model character to investigate the interplay of orbital phenomena with magnetism. Here we present an experimental and theoretical investigation of multipolar collective excitation modes in the hidden order state of CeB_6. Both low- and high-energy modes are observed with inelastic neutron scattering in fields up to 16.5 T. Their position, field strength and angle dependence is compared to the results of a multipolar interaction model, calculated within a localized approach using the pseudo-spin presentation of the fourfold degenerate Γ_8 crystalline electric field ground state.

Critical dynamics in Ca_2RuO_4 studied by neutron resonant spin-echo spectroscopy

Matthias Hepting (Max-Planck-Institute (MPI) for Solid State Research)

Tuesday, 16:15

Heiko Trepka (Max-Planck-Institute (MPI) for Solid State Research), Juan Porras (Max-Planck-Institute (MPI) for Solid State Research), Maximilian Krautloher (Max-Planck-Institute (MPI) for Solid State Research), Thomas Keller (Max-Planck-Institute (MPI) for Solid State Research), Bernhard Keimer (Max-Planck-Institute (MPI) for Solid State Research)

We have used the spin-echo capabilities of TRISP at FRM II to determine the linewidth of critical antiferromagnetic fluctuations in Ca_2RuO_4 (CRO) above the Néel temperature. CRO hosts a complex interplay between magnetic and electronic correlations, and exhibits 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 [1]. However, the nature of the electronic order in CRO above the Néel temperature is still under debate and the emergence of an exotic spin-nematic or an orbitally ordered state have been proposed [2,3]. Since the magnetic fluctuations are fundamentally related to the nature of the magnetism, with the magnetic order parameter possibly coupling to the electronic states, our investigation of the critical magnetic scattering might help to clarify the type of the electronic order in CRO.

[1] A. Jain et al., Nat. Phys. 13, 633 (2017).

[2] H. Liu and G. Khaliullin, Phys. Rev. Lett. 122, 057203 (2019).

[3] I. Zegkinoglou et al., Phys. Rev. Lett. 95, 136401 (2005).

click here to go to first page of this workshop

Quantum Phenomena III

Tuesday – December 10th, 2019
17:00-18:00

17:00 - 17:30	**Magnetic Nanoparticle Spin Structures**	*Sabrina Disch*
17:30 - 17:45	**Exchange interactions at the manganite/manganite interface of FM/AFM type**	*Laura Guasco*
17:45 - 18:00	**Neutron Depolarization Measurements of Quantum Critical Ferromagnets**	*Marc Seifert*

Magnetic Nanoparticle Spin Structures

Sabrina Disch (University of Cologne)

Tuesday, 17:00

Magnetic nanoparticles reveal unique magnetic properties which make them relevant for data storage, electronic and mechanical engineering, and biomedical applications. Whereas the implementation of nanomagnetic properties into technological applications is progressing rapidly, understanding the microscopic origin of phenomena such as size-dependent magnetization and magnetic anisotropy is fundamentally challenging and needs intensive research.

In this talk, I will present recent examples of our research into the spin structure of nanoparticles on different scales. First, the nanoscale spin structure of ferrite nanoparticles will be addressed as obtained from polarized SANS. Longitudinal polarization analysis reveals the existence of spin disorder or spin canting, responsible for the low magnetization in nanoparticles as compared to the bulk material. The second focus will be on the size evolution of atomic scale, spin spiral magnetic ordering in cobalt chromite nanoparticles [1,2]. Using polarized neutron diffraction with XYZ polarization analysis, we have established critical coherent domain sizes for the formation of the spin spiral and ferrimagnetic structure and revealed the evolution of the incommensurate spin spiral vector with particle size.

[1] D. Zákutná, S. Disch et al., Phys. Rev. B 98 (2018) 064407.

[2] D. Zákutná, S. Disch et al., arXiv:1908.10582 (2019).

Exchange interactions at the manganite/manganite interface of FM/AFM type

Laura Guasco (Max-Planck Institute (MPI) for Solid State Research)

Tuesday, 17:30

Yury Khaydukov (Max-Planck Institute (MPI) for Solid State Research), Gideok Kim (Max-Planck Institute (MPI) for Solid State Research), Thomas Keller (Max-Planck Institute (MPI) for Solid State Research, Outstation at MLZ), Gennady Logvenov (Max-Planck Institute (MPI) for Solid State Research), Alexei Vorobiev (Department of Physics and Astronomy, Uppsala University), Peter Wochner (Max-Planck Institute (MPI) for Solid State Research), Bernhard Keimer (Max-Planck Institute (MPI) for Solid State Research)

Understanding interface phenomena is one of the greatest challenges in both fundamental and applied physics. In particular, interfaces made of strongly correlated oxides have shown unexpected physical properties, such as the exchange bias, proximity effects, charge transfer, exchange springs and orbital reconstruction [1-3]. Given the complexity of its structural and magnetic phase diagram, LSMO offers a wide range of tunable properties that we can stack into heterostructures. With the atomic precision of the oxide MBE we were able to tune the Sr-concentration x layer by layer (at 0.4 obtaining a ferromagnetic half-metal and at 0.8 an antiferromagnetic insulator), and synthesize superlattices with a large gradient in hole doping, as a promising platform to study the competition between diverse exchange interactions, such as exchange bias and charge transfer.

In this talk, we will discuss the results obtained by polarized neutron reflectometry and SQUID magnetometry of these heterostructures, while trying to shed light on the macroscopic and local magnetic properties and their connection to the Sr-doping depth profile.

[1] Jason D. Hoffman et al., Phys. Rev. X 6, 041038 (2016)

[2] J.-H. Kim, I. Vrejoiu, Y. Khaydukov, T. Keller, J. Stahn, A. Rühm, D. K. Satapathy, V. Hinkov, and B. Keimer, Phys. Rev. B 86, 180402(R)

[3] J. Stahn, et al., Phys. Rev. B 71, 140509(R), (2005)

Neutron Depolarization Measurements of Quantum Critical Ferromagnets

Marc Seifert (Department of Physics, Technical University of Munich)

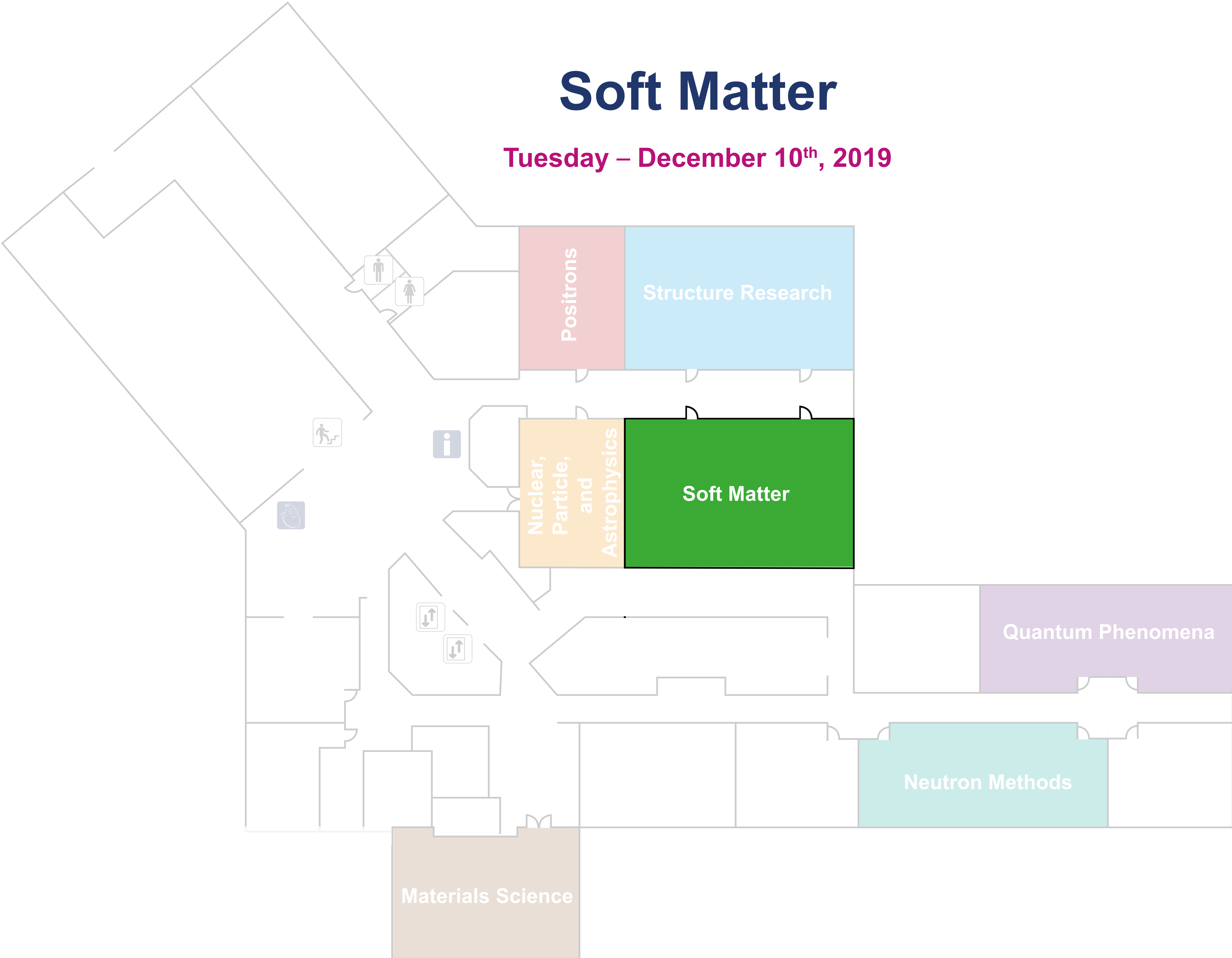
Tuesday, 17:45

Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich) Pau Jorba (Department of Physics, Technical University of Munich), Andreas Bauer (Department of Physics, Technical University of Munich), James Schilling (Department of Physics, Technical University of Munich), Christian Pfleiderer (Department of Physics, Technical University of Munich)

In ferromagnetic quantum critical systems it is possible to suppress the Curie temperature to 0 K by changing an external control parameter such as a magnetic field or hydrostatic pressure. Recent theories suggest a generic phase diagram for clean quantum critical ferromagnets featuring a tricritical point where the order of the phase transition changes from 2nd to 1st. This behavior has already been observed e.g. in $ZrZn_2$ and MnSi, and is also discussed for $SrRuO_3$. An exception to this behavior could be the ferromagnetic Kondo lattice CePt as no tricritical point was observed, yet. The neutron depolarization technique offers new insight into ferromagnetic quantum critical systems as it enables us to directly probe ferromagnetism in challenging sample environments, such as magnetic fields, low temperatures, and high pressures. We present two neutron depolarization studies of the compounds $SrRuO_3$ and CePt up to hydrostatic pressures of 17 GPa and 12 GPa, respectively.

Soft Matter

Tuesday – December 10th, 2019



click here to go to first page of this workshop

Soft Matter I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:40	**Neutron Invisible detergents for solution structure determination of membrane proteins by Small-Angle Neutron Scattering** *Lise Arleth*
13:40 - 14:05	**All-in-one “schizophrenic” self-assembly of orthogonally tuned thermoresponsive diblock copolymers** *Christine Papadakis*
14:05 - 14:30	**Structural Properties of Micelles formed by Telechelic Pentablock Quaterpolymers with pH-responsive Midblocks and Thermo-responsive End Blocks in Aqueous Solution** *Florian Jung*

Neutron Invisible detergents for solution structure determination of membrane proteins by Small-Angle Neutron Scattering

Lise Arleth (Niels Bohr Institute, University of Copenhagen)

Tuesday, 13:00

We recently showed how stealth detergents, which are detergents where the H/D balance are head and tail groups are individually tuned to make them invisible to neutrons, could be synthesized and generally applied as a method for determining structures of membrane proteins in solution via small-angle neutron scattering (SANS) (1). With these stealth detergents, only the signal from the membrane protein remained in the SANS data. We demonstrated that the method was generally applicable for low-resolution structural investigations of membrane proteins by evaluating five very different membrane proteins (1,2). Recently we also showed how Size-Exclusion Chromatography could be directly coupled to SANS to yield a “SEC-SANS” setup that provided strongly improved sample quality of these challenging samples (3). By combining the two developments we obtain an experimental approach that improves solution structure determination of membrane proteins by SANS and simplifies the subsequent data analysis. We have used the approach to investigate different structural hypotheses for membrane proteins and I will show recently obtained and somewhat puzzling data from the pentameric magnesium transporter CorA to illustrate this.

[1] Midtgaard et al, FEBS Journal, 2018, 285(2) 357-371.

[2] Larsen et al, IUCR Journal, 2018, 5(6), 780-793.

[3] Johansen et al, Acta Cryst D, 2018, 74(12), 1178-1191.

All-in-one “schizophrenic” self-assembly of orthogonally tuned thermoresponsive diblock copolymers

Christine Papadakis (Department of Physics, Technical University of Munich)

Tuesday, 13:40

Natalya Vishnevetskaya (Department of Physics, Technical University of Munich), Viet Hildebrand (Institut für Chemie, Universität Potsdam), Noverra M. Nizardo (Institut für Chemie, Universität Potsdam), Chia-Hsin Ko (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich), André Laschewsky (Institut für Chemie, Universität Potsdam, and Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm)

Smart, fully orthogonal switching was realized in a diblock copolymer system with variable trigger-induced aqueous self-assembly. The polymers are composed of nonionic and zwitterionic blocks featuring lower and upper critical solution temperatures (LCSTs and UCSTs). In the system investigated, diblock copolymers from poly(N-isopropyl methacrylamide) (PNIPMAM) and a poly(sulfobetaine methacrylamide), variation of the molar mass of the latter block shifts its UCST above the LCST of the PNIPMAM block in a salt-free condition. Successive thermal switching results in “schizophrenic” micellization, in which the roles of the hydrophobic core block and the hydrophilic shell block are interchanged [1]. Adding salt, the UCST is shifted below the LCST of the PNIPMAM block by adding small amounts of a salt, thus inverting the pathway of switching. Small-angle neutron scattering was used to verify that this orthogonal switching by electrolyte addition results in two switching scenarios between the two types of micelles, namely (i) via an insoluble state or (ii) via a molecularly dissolved state. The versatile and tunable self-assembly offers manifold opportunities, for example, for smart emulsifiers or for sophisticated carrier systems.

[1] N. S. Vishnevetskaya, C. M. Papadakis et al., Macromolecules 49, 6655 (2016), 50, 3985 (2017) and 51, 2604 (2018), Langmuir 35, 6441 (2019). C. M. Papadakis, P. Müller-Buschbaum, A. Laschewsky, Langmuir 35, 9660 (2019).

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

Florian Jung (Department of Physics, Technical University of Munich)

Tuesday, 14:05

Panayiota A. Panteli (Department of Chemistry, University of Cyprus), Chia-Hsin Ko (Department of Physics, Technical University of Munich), Jia-Jhen Kang (Technical University of Munich), Lester Barnsley (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Constantinos Tsitsilianis (Department of Chemical Engineering, University of Patras, Costas S. Patrickios (Department of Chemistry, University of Cyprus), Christine Papadakis (Department of Physics, Technical University of Munich)

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 thermo-responsive 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(nBuMA$_8$-co-TEGMA$_8$)-b-PDMAEMA$_{50}$-b-PEG$_{46}$-b-PDMAEMA$_{50}$-b-P(nBuMA$_8$-co-TEGMA$_8$) 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 they are stabilized at low pH values. In summary, the micelles show complex responsive behavior in dependence on temperature and the pH value.

click here to go to first page of this workshop

Soft Matter II

Tuesday – December 10th, 2019
15:00-16:30

15:00 - 15:40	**Coupling between protein and hydration water dynamics** *Martin Weik*
15:40 - 16:05	**Ternary complex formation and photoactivation of a photoenzyme results in altered protein structure and dynamics** *Andreas Stadler*
16:05 - 16:30	**Phase transition kinetics in a doubly thermo-responsive block copolymer thin film** *Lucas Kreuzer*

Coupling between protein and hydration water dynamics

Martin Weik (Institut de Biologie Structurale (ibs))

Tuesday, 15:00

The combination of incoherent neutron scattering (INS) and selective deuterium labelling is a powerful tool that puts the focus either on protein or on water motions on the ns-ps time scale and allows their dynamic coupling to be studied (Schiro et al. (2015) Nat Com 6, 6490). We have started focusing on the hydration-water dynamics of those proteins that can form the pathological fibers involved in so-called protein aggregation diseases, such as the intrinsically disordered proteins tau (Alzheimer's) and α-synuclein (Parkinson's). So far, evidence has been found that hydration water mobility is enhanced around tau amyloid fibers, a finding that identifies hydration water entropy as a potentially universal driving force behind fiber formation (Fichou et al. (2015) PNAS 112, 6365). Recently, we extended our study to α-synuclein and combined INS on SPHERES (MLZ) with molecular dynamics simulations on full-length monomers and fibers (Pounot, Forsyth, Härtlein, Langkilde, Marasini, Moulin, Schiro, Seydel, Tobias, Vestergaard, Weik, Zamponi, unpublished). Ongoing efforts aim at following changes in protein dynamics during fiber formation in situ by time-resolved neutron backscattering. A proof-of-principle study on lysozyme was successfully carried out on IN16B (ILL) and shows that the apparent diffusion coefficient decreases monotonically during fiber formation, whereas internal protein dynamics remain unchanged (Pounot, Chaaban, Fodera, Schiro, Seydel, Weik, unpublished).

Ternary complex formation and photoactivation of a photoenzyme results in altered protein structure and dynamics

Andreas Stadler (Jülich Centre for Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH)

Tuesday, 15:40

Judith Schneidewind (Heinrich-Heine-Universität Düsseldorf), Michaela Zamponi (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Esther Knieps-Grünhagen (Heinrich-Heine-Universität Düsseldorf), Samir Gholami, Ulrich Schwaneberg (RWTH Aachen), Ivan Rivalta (Universitá de Bologna), Marco Garavelli (Universitá de Bologna), Mhedi Davari (RWTH Aachen), Karl-Erich Jaeger (Institute of Molecular Enzymtechnology, Heinrich-Heine-Universität Düsseldorf, Outstation at Forschungszentrum Jülich GmbH), Frank Krause, Marco Bocola, Ulrich Krauss (Heinrich-Heine-Universität Düsseldorf)

The interplay between protein dynamics and catalysis remains a fundamental question in enzymology. Here, we investigate the ns-timescale dynamics (1) and solution structures (2) of a light-dependent NADPH: protochlorophyllide oxidoreductase (LPOR), a photoenzyme crucial for chlorophyll synthesis. Due to the lack of an LPOR structure, the global structural and dynamic consequences of LPOR/Pchlide/NADPH ternary complex formation remained elusive up to now. By employing quasielastic neutron scattering (QENS) we show that the formation of the ternary holoprotein complex as well as photoactivation lead to progressive rigidification of the protein. Molecular dynamics (MD) simulations, in good agreement with the experimental QENS results, suggests that the increased flexibility observed for the apoprotein stems from structural fluctuations of the NADPH and Pchlide substrate binding sites of the enzyme. In addition, we investigated structural properties of the apo and holoproteins using MD simulations, multi-wavelength analytical ultracentrifugation (MWA-AUC) and small angle X-ray scattering (SAXS) experiments to build a consensus model of the LPOR apoprotein and the substrate/cofactor/LPOR ternary complex. Our findings advance the structural and dynamic understanding of LPORs and provide a first link between protein dynamics and catalysis for this enzyme class.

[1] Stadler et al. J. Phys. Chem. B, 2019, 123, 34, 7372-7384

[2] Schneidewind et al. Communications Biology, accepted.

Phase transition kinetics in a doubly thermo-responsive block copolymer thin film

Lucas Kreuzer (Department of Physics, Technical University of Munich)

Tuesday, 16:05

Tobias Widmann (Department of Physics, Technical University of Munich), Lorenz Bießmann (Department of Physics, Technical University of Munich), Raphael Märkl (Department of Physics, Technical University of Munich), Jean-Francois Moulin (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Viet Hildebrand (Institut für Chemie, Universität Potsdam), André Laschewsky (Institut für Chemie, Universität Potsdam, and Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm), Christine Papadakis (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Thermo-responsive polymers respond to small changes in temperature with a drastic change in their conformation, which makes them promising candidates for manifold application fields. While the underlying mechanisms of such polymers in solution are well understood, less is known about thermo-responsive polymers in thin film morphology. In our recent work, we follow the phase transition kinetics upon increasing temperature in-situ in a doubly thermo-responsive block copolymer thin film. The block copolymer consists of a poly(N-isopropylmethacrylamide) (PNIPMAM) block, which shows a lower critical solution temperature (LCST) and a zwitterionic poly(sulfobetaine) (PSPP) block, which exhibits an upper critical solution temperature (UCST) that is lower than the corresponding LCST of the PNIPMAM block. At temperatures below the UCST, the polymer film is swollen in D2O atmosphere in order 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). The kinetic processes (swelling and temperature jumps) are followed with via time-of-flight neutron reflectometry (TOF-NR) with high time resolution. Static TOF-NR measurements and TOF grazing incidence small angle neutron scattering (GISANS) measurements are performed at the beginning and in between the kinetic processes to gain a complete picture of the swelling and temperature-dependent behavior of the polymer thin film.

Soft Matter III

Tuesday – December 10th, 2019
13:00-14:30

17:00 - 17:25	**Rheo-VSANS: application to polydisperse micron-sized colloidal particles** *Akira Otsuki*
17:25 - 17:50	**Operando SANS for gaining potable water via reverse osmosis desalination – exploration of colloidal silica fouling** *Dietmar Schwahn*
17:50 - 18:00	**Summary**

click here to go to first page of this workshop

Rheo-VSANS: application to polydisperse micron-sized colloidal particles

Akira Otsuki (University of Lorraine)

Tuesday, 17:00

This paper reports the series of developments and investigations on in situ coupling of rheology with very small-angle neutron scattering (rheo-VSANS) measurements of polydisperse colloidal particle suspensions. This coupling allows us to directly correlate microscopic particle-particle interaction with macroscopic suspension behavior under different physical and chemical environments. In this paper, aqueous suspensions composed of colloidal particles, including metal oxide particles, are introduced as examples. The research gaps are identified and specific future perspectives are discussed to further enhance the use of this useful coupling, and its application toward the transition from the evaluation of simple particle suspension systems to more complex particle suspension systems that fit more with the interest and needs of particle processing industries.

Operando SANS for gaining potable water via reverse osmosis desalination – exploration of colloidal silica fouling

Dietmar Schwahn (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

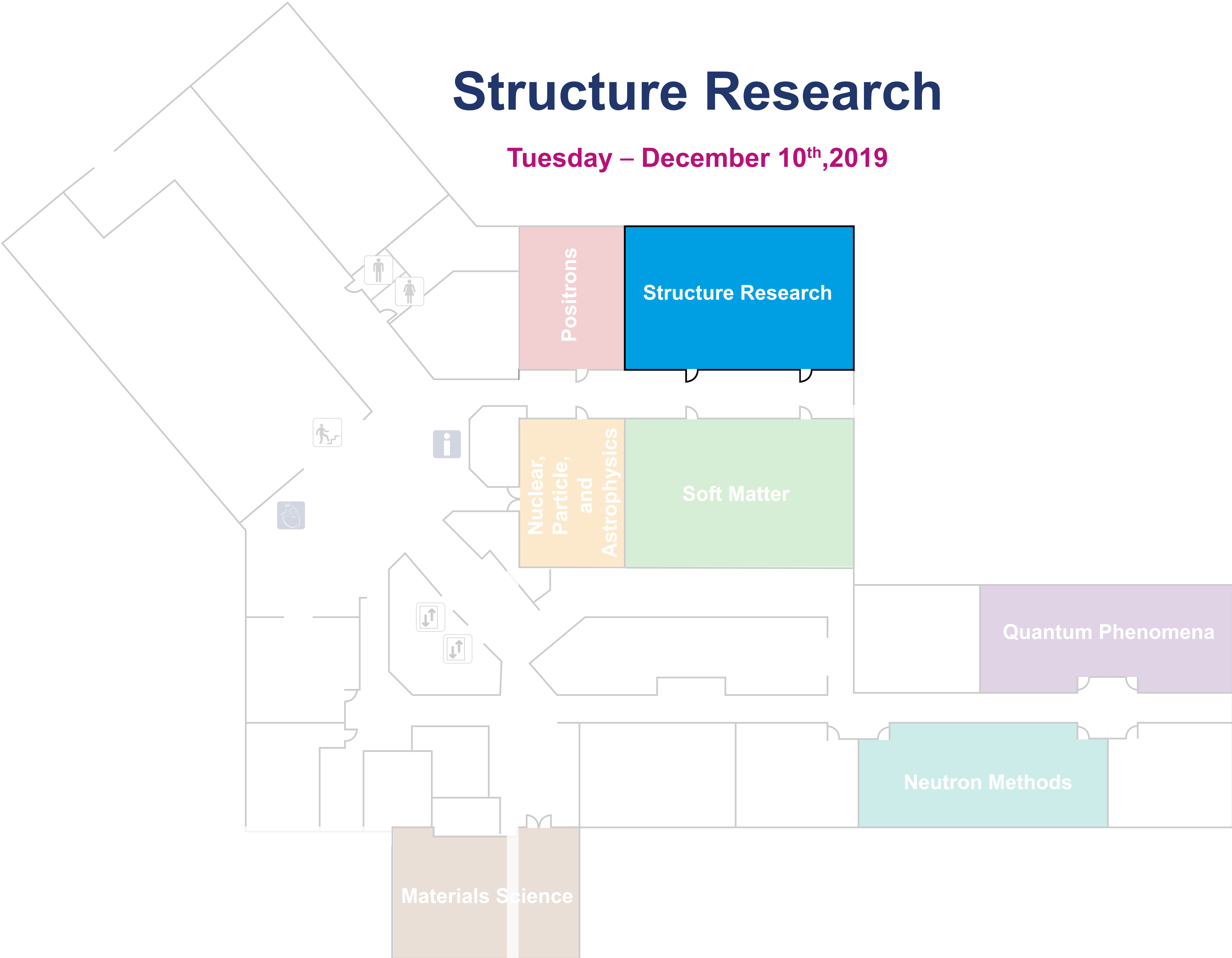
Tuesday, 17:25

Vitaliy Pipich (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Winfried Petry (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Operando SANS experiments of reverse osmosis (RO) desalination gaining potable water from sea and wastewater have been realized by us. Two cells are designed for pressure up to 50 bars and a tangential cross-flow of the feed up to 36 L/h. One cell is equipped with a membrane whereas the other cell is not (EC, empty cell) to measure the feed solution alone. Basically, we will present fouling experiments of inorganic silica nanoparticles, a topic which is intensely discussed in literature. Silica of 250 Å radius and 1.09 % volume fraction (ionic strength 10 mM) were dissolved in water (feed solution). Essential results are observation of a reflection peak of a simple cubic lattice representing a so-called cake layer on top of the membrane. The peak is continuously increasing and slightly shifting to larger Q indicating compaction of the cake layer. The distance of the silica colloids evaluated from the peak position Qm corresponds with their diameter. Another relevant parameter is the silica volume fraction at three positions of the RO devise, namely away from the membrane in the EC, in front of the membrane and of the cake layer. From the cake layer concentration we estimate a thickness of the cake layer, which increases from 4 to 16 micron when considering the silica volume fraction of simple cubic crystals as 52 vol%. The silica volume fraction shows about a twice larger value in front of the membrane than in the EC indicating strong concentration polarization.

Structure Research

Tuesday – December 10th,2019



Structure Research I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:30	**Overview of the existing diffraction capabilities at MLZ and future prospects** *Anatoliy Senyshyn, Martin Meven*
13:30 - 14:00	**Ligand Protonation and Changes of the Water Inventory Determined by High-Resolution Neutron Structures upon Trypsin Complex Formation** *Andreas Heine*
14:00 - 14:30	**Our crystal structure investigations using SPODI** *Florian Kraus*

Overview of the existing diffraction capabilities at MLZ and future prospects

Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich),
Martin Meven (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Tuesday, 13:00

Single crystal and/or powder diffraction are the experimental techniques, which stands on the forefront of the material characterisation, delivering the key information about the crystal structure, symmetry and chemical contentn. Being perfectly parametrized and standardized technique, the diffraction is widely used and an X-ray powder diffractometer is a part of equipment in nearly every lab specializing on materials preparation and research.

Neutron diffraction as a result of combining diffraction strengths with the well-known advantages of neutrons provide unique structural information, complementary to X-ray or electron diffraction. The diffractometers serve as working horses at any Large Scale Facility. In the current contribution the Overview of the available diffraction capabilities at MLZ will be made with a special focus on the future prospects and developments.

Ligand Protonation and Changes of the Water Inventory Determined by High-Resolution Neutron Structures upon Trypsin Complex Formation

Andreas Heine (Institute of Pharmaceutical Chemistry, Philipps-University Marburg)

Tuesday, 13:30

Johannes Schiebel (Philipps-University Marburg), Tobias Schrader (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Andreas Ostermann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Gerhard Klebe (Philipps-University Marburg)

Hydrogen atoms are usually neglected in protein structures due to experimental difficulties in their detection; nevertheless, they play an important role in ligand recognition and protonation states of ligand and protein. In hydrogen-bond interactions, and as part of water molecules, hydrogen atoms indicate the geometry of hydrogen-bonding networks and help to classify the rotational states of water molecules in protein environments. High resolution neutron diffraction enables the detection of hydrogen atoms and thus allows to address the above mentioned points. We determined exceptionally high resolution neutron structures (better than 1.45Å) of trypsin in its apo state and in complex with a series of similar, small molecule ligands. These structures were complemented with corresponding high resolution X-ray structures. At first, we investigated binding of the structurally related molecules aniline and 2-aminopyridine to trypsin. Neutron structures revealed different protonation patterns of the two ligands and indicate a large Ka shift for aniline.[1] In a second study, we investigated the water structure of uncomplexed trypsin and corresponding changes upon benzamidine and N-amidinopiperidine binding. Observed changes in the solvation pattern and ordering states of water molecules might give an explanation for the strength of inhibitor binding.[2]

[1] Schiebel, J. et al. (2017) Angew. Chem. Int. Ed. 56, 4887-4890.
[2] Schiebel, J. et al. (2018) Nat. Commun. 9, 3559.

Our crystal structure investigations using SPODI

Florian Kraus (Philipps-Universität Marburg)

Tuesday, 14:00

Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Martin Mühlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Sergei Ivlev (Philipps-Universität Marburg)

We will present our crystal structure determinations of various chemical compounds synthesized by us during our investigations in the fields of beryllium, uranium and fluorine chemistry. Neutron diffraction on powders provided crucial insights, for example for hydrogen bonding and precise positioning of light atoms close to heavy ones. The synthesis and crystal structures of $Be(ND_3)_4Cl_2$,[1] $Ba(BrF_4)_2$,[2] NaF·nHF (n = 2, 3, 4),[3] $UCl_4(HCN)_4$,[4] $Mn(ND_3)_6(N3)_2$,[5] α- and β-F_2,[6] and α- and β-NF_3 will be presented.[7]

[1] F. Kraus, S. A. Baer, M. Hoelzel, A. J. Karttunen, Eur. J. Inorg. Chem. 2013, 2013, 4184–4190.

[2] S. Ivlev, V. Sobolev, M. Hoelzel, A. J. Karttunen, T. Müller, I. Gerin, R. Ostvald, F. Kraus, Eur. J. Inorg. Chem. 2014, 2014, 6261–6267.

[3] S. I. Ivlev, T. Soltner, A. J. Karttunen, M. J. Mühlbauer, A. J. Kornath, F. Kraus, Z. Anorg. Allg. Chem. 2017, 643, 1436–1443.

[4] S. S. Rudel, C. Pietzonka, M. Hoelzel, F. Kraus, Chem. Commun. 2018, 54, 1241–1244.

[5] S. I. Ivlev, T. G. Müller, A. J. Karttunen, M. Hoelzel, F. Kraus, Z. Anorg. Allg. Chem. 2018, 644, 1349–1353.

[6] S. I. Ivlev, A. J. Karttunen, M. Hoelzel, M. Conrad, F. Kraus, Chem. - Eur. J. 2019, 25, 3310–3317.

[7] S. I. Ivlev, M. Conrad, M. Hoelzel, A. J. Karttunen, F. Kraus, Inorg. Chem. 2019, 58, 6422–6430.

Structure Research II

Tuesday – December 10th, 2019
13:00-14:30

15:00 - 15:30	**How neutron diffraction helps to understand ionic conduction in solids** *Wolfgang Zeier*
15:30 - 15:50	**Time- and space information of proton dynamics in hydrogen bond networks in $Fe^{2+}Fe^{3+}_{3.2}(Mn^{2+},Zn)_{0.8}(PO_4)_3(OH)_{4.2}(HOH)_{0.8}$** *Sohyun Park*
15:50 - 16:10	**Polarized neutron diffraction studies on weak ferromagnets at instrument POLI at MLZ** *Henrik Thoma*
16:10 - 16:30	**Realization of kagome spin ice state in an intermetallic compound** *Hao Deng*

How neutron diffraction helps to understand ionic conduction in solids

Wolfgang Zeier (Justus-Liebig-University Giessen)

Tuesday, 15:00

The advent of solid-state batteries has spawned a recent increase in interest in lithium conducting solid electrolytes, especially in the lithium thiophosphates. However, often the underlying principles governing the ionic transport are not known.

In this presentation, we will discuss two of our recent approaches to understand the underlying structures of some ionic conductors and optimizing their ionic conductivities in order to identify an ideal solid electrolyte for SSBs. First, we will show how neutron diffraction studies help to elucidate the diffusion pathways in the solid electrolyte $Li_{10}GeP_2S_{12}$ and how neutron diffraction is used to corroborate the existence of inductive effects. Second, we will show our recent attempts to understand the ionic conduction principles in the lithium argyrodites Li_6PS_5X. Using neutron diffraction, the lithium substructure is probed and influenced by structural disorder.

Time- and space information of proton dynamics in hydrogen bond networks in $Fe^{2+}Fe^{3+}_{3.2}(Mn^{2+},Zn)_{0.8}(PO_4)_3(OH)_{4.2}(HOH)_{0.8}$

Sohyun Park (Ludwig-Maximilians-Universität Munich (LMU))

Tuesday, 15:30

Wiebke Lohstroh (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Peter Lunkenheimer (Experimental Physics V Center for Electronic Correlations and Magnetism, University of Augsburg), Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The time and length scales for fast proton dynamics in several ps over hydrogen bonds (HBs) in the title compound could be determined from quasi-elastic neutron scattering (QENS) at TOFTOF. Its dielectric response in a wide frequency range of 1 Hz - 3 GHz from 30 K to 500 K is implicated in its structural properties revealed by Rietveld refinements using neutron powder diffraction data (SPODI). The evolution of three distinct phonons in an energy range of -15 meV and -50 meV from 250 K to 400 K detected in QENS can be addressed to collective motions of the framework polyhedra as OH and HOH groups form their ligands with oxygens. Two distinctly decoupled proton dynamic processes occur in this system: at high temperatures, global protonic transport is thermally activated over an energy barrier (EB) of 0.49 eV. At low temperatures, relaxational proton hopping between double-well potentials in HBs is activated at EB = 0.62 eV. An extremely fast relaxation time in several ps continuously slows down to ~100 s before the entrance into an orientational proton-glass state at about 125 K. Isosurface of bond valence energy landscape maps of H+ at 0.49 eV clearly evidence the honeycomb-shaped route for the protonic conductivity at 393 K, which accords with neutron scattering length densities reconstructed by the Maximum-Entropy Method.

click here to go to first page of this workshop

Polarized neutron diffraction studies on weak ferromagnets at instrument POLI at MLZ

Henrik Thoma (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Tuesday, 15:50

Vladimir Hutanu (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Polarized neutron diffraction (PND) is a powerful method to investigate magnetic structures. PND can be used for very precise magnetization measurements even for weak magnetic contributions. It allows the high-quality determination of magnetic form factors, to untangle complex (e.g. chiral) magnetic structures, and to follow the movement of magnetic domains. By conserving the phase relation between the nuclear and magnetic structure, this technique is also a valuable tool to investigate the Dzyaloshinskii–Moriya interaction (DMI) [1], which is an important driving force in many magnetic materials including weak ferromagnets.

Using the Flipping Ratio (FR) setup [2] of POLI [3] at MLZ, the magnetic structures of two prototypical weak ferromagnets, hematite (α-Fe_2O_3) and rhodochrosite ($MnCO_3$), have been studied in detail as function of the applied magnetic field and temperature. This allowed us to determine the magnetic susceptibility tensor and, for the first time with neutrons, the absolute sign of the DMI in both compounds. Moreover, due to the large q-range access of POLI, we were able to reconstruct field induced magnetization density distribution maps by using the maximum entropy method.

[1] V. E. Dmitrienko et al., Nat. Phys. 10, 202 (2014)

[2] H. Thoma, W. Luberstetter, J. Peters, and V. Hutanu, J. Appl. Cryst. 51, 17-26 (2018)

[3] V. Hutanu, Heinz Maier-Leibnitz Zentrum, Journal of large-scale research facilities, 1, A16 (2015)

Realization of kagome spin ice state in an intermetallic compound

Hao Deng (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Tuesday, 16:10

Kan Zhao (Experimentalphysik VI, Center for Electronic Correlations and Magnetism, University of Augsburg), Vladimir Hutanu (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Spin ices are exotic phases of matter characterized by frustrated spins obeying local ice rules that minimize the number of spatially isolated magnetic monopoles, in analogy with the electric dipoles in water ice. In two dimensions, one can similarly define ice rules for inplane Ising-like spins arranged on a kagome lattice, which require each triangle plaquette to have a single monopole, and can lead to various unique orders and excitations. By integral experimental and theoretical approaches including magnetometry, thermodynamic measurements, neutron scattering and Monte Carlo simulations, we establish HoAgGe as the first crystalline (i.e. non-artificial) system to realize kagome spin ice state. It features a variety of partial and fully ordered states and sequence of field-induced phases at low temperatures, all consistent with the kagome ice rule.

Structure Research III

Tuesday – December 10th, 2019
17:00-18:00

17:00 - 17:30	**On the Dzyaloshinsky-Moria interaction in RMn_2O_5 multiferroics**	*Igor Zobkalo*
17:30 - 17:50	**Combined X-ray and neutron single-crystal diffraction in diamond anvil cells**	*Andrzej Grzechnik*
17:50 - 18:00	**Summary**	

On the Dzyaloshinsky-Moria interaction in RMn_2O_5 multiferroics

Igor Zobkalo (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre «Kurchatov Institute»)

Tuesday, 17:00

Vladimir Hutanu (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ)), Andrew Sazonov, Anna Matveeva (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre «Kurchatov Institute»)

Manganite oxides family RMn_2O_5 (R – rare-earth element) represents prominent example of a multiferroics with extremely interesting and close relationship between magnetism and ferroelectricity. The understanding of the microscopic mechanisms responsible for spin-driven ferroelectricity in these compounds considered to be the actual and intriguing issue in the studies of multiferroicity of magnetic origin. In order to make a new approach to clarifying those mechanisms we performed the detailed investigations of the magnetic ordering in single crystals of multiferroics $Nd_{1-x}Tb_xMn_2O_5$ (x = 0, 0.2, 1) using both non-polarized and polarized neutron diffraction techniques.

We show that in all the crystals the chiral scattering originated from the difference between the population of right- and left-handedness chiral domains was observed. This difference can be controlled by the external electric field of few kV/cm revealing strong magnetoelectric coupling. The results are considered within the frames of antisymmetric super-exchange model for Dzyaloshinsky-Moria interaction.

Combined X-ray and neutron single-crystal diffraction in diamond anvil cells

Andrzej Grzechnik (RWTH Aachen)

Tuesday, 17:30

Martin Meven (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ)), Karen Friese (Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4),- Forschungszentrum Jülich GmbH)

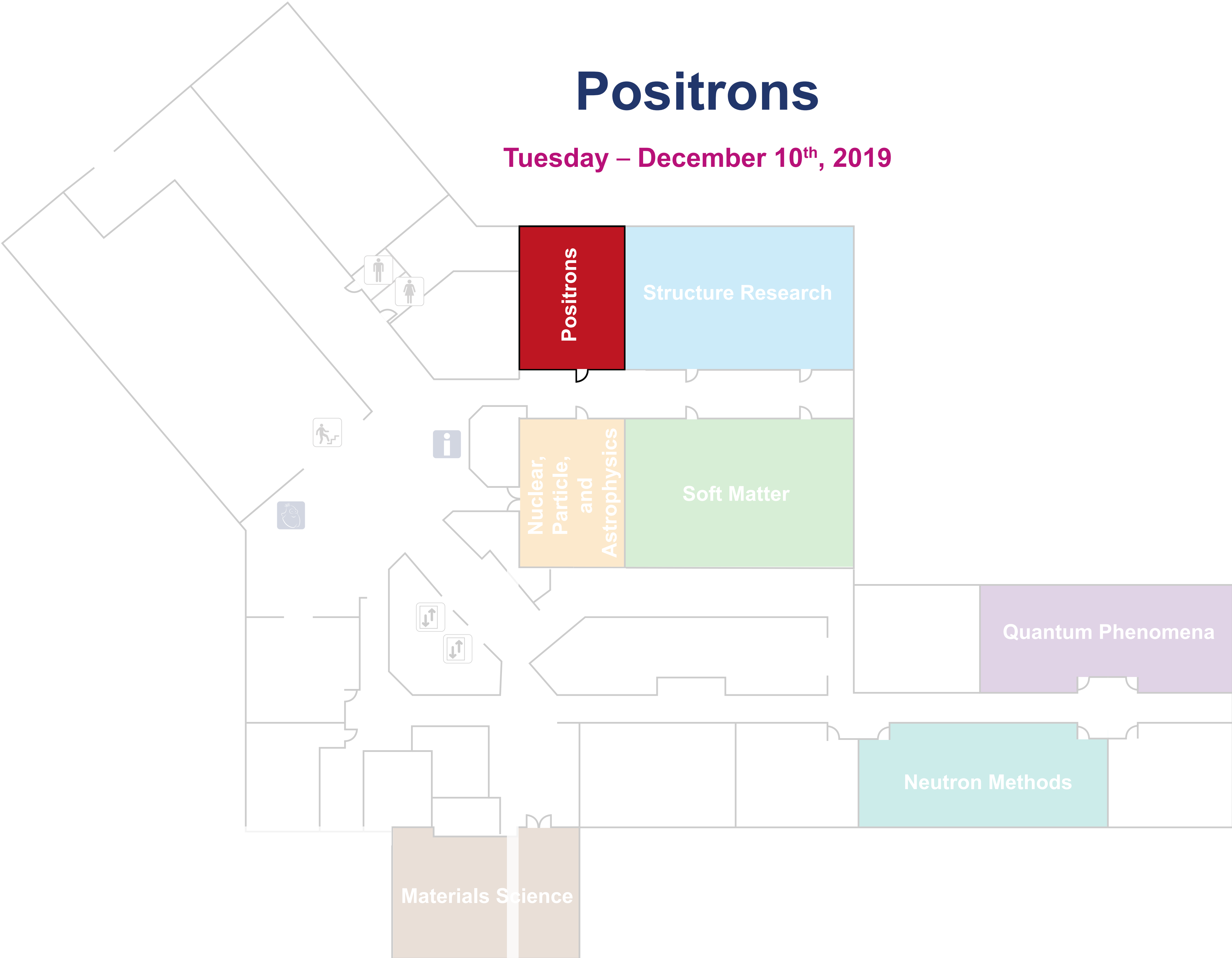
Owing to the tremendous development of radiation sources and area-sensitive detectors, single-crystal X-ray diffraction in diamond anvil cells (DAC) can now be performed on complex crystal structures to megabar pressures. However, there are hardly any single-crystal neutron diffraction studies in the DAC that would present complete structural refinements. The reason is that it is still difficult to study crystals with volumes below 1 mm^3 due to the low flux of the neutron beams. The requirement for large samples hinders a combined use of X-ray and neutron single-crystals diffraction upon compression. The combination of both techniques is advantageous as neutron diffraction plays a crucial role in cases where X-ray diffraction fails to provide information on, for instance, magnetic (dis)order or hydrogen bonding.

We have developed transmission cells for both neutron and X-ray single-crystal diffraction. One of them is equipped with a membrane filled with the He gas that could be operated remotely. The same crystal in the same DAC can now be studied on laboratory X-ray diffractometers, synchrotron beamlines, and at neutron facilities. We have also worked out proper procedures to combine the neutron and X-ray data for joint refinements of the crystal structure.

We are now producing a new transmission DAC made of the Ni-Cr-Al alloy with very large opening angles that would allow a wider access to the reciprocal space, close to the one in our panoramic diamond anvil cell.

Positrons

Tuesday – December 10th, 2019



Positrons I

Tuesday – December 10th, 2019
13:00-14:30

13:00 - 13:15	**Status of the Positron Beam Facility and New Developments at NEPOMUC** *Christoph Hugenschmidt*
13:15 - 13:40	**Vacancy-type defects in ion-implanted GaN probed by monoenergetic positron beams** *Akira Uedono*
13:40 - 14:05	**Evolution of vacancies in thin film solar cells and in photochromic yttrium oxyhydride revealed by in-situ positron annihilation spectroscopy** *Stephan Eijt*
14:05 - 14:30	**The pulsed positron beams PLEPS and SPM for defect profiling with positron lifetime measurements at NEPOMUC: applications and developments** *Werner Egger*

Status of the Positron Beam Facility and New Developments at NEPOMUC

Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Tuesday, 13:00

The neutron induced positron source NEPOMUC at FRM II/MLZ provides the world's highest intensity of 10^9 moderated positrons per second. The primary energy of the positrn beam is set to 1 keV. For the vast majority of user experiments, however, the brightness enhanced remoderated positron beam with a typical energy of 20 eV (~$5x10^7$ positrons per second) is used.

Within this contribution features of the positron beam provided by NEPOMUC and technical upgrades of the positron beam facility such as the improved remoderator stage and new high. stability power supplies for both, electric lenses and magnetic field coils for positron beam transport will be presented. An overview of current and future developments of positron instrumentation will be given. Finally, various options of positron beam experiments, which are planned to be operated in the neutron guide hall east in the long term, will be discussed.

Vacancy-type defects in ion-implanted GaN probed by monoenergetic positron beams

Akira Uedono (University of Tsukuba)

Tuesday, 13:15

Werner Egger (Universität der Bundeswehr München), Tönjes Koschine (Universität der Bundeswehr München), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Marcel Dickmann (Universität der Bundeswehr München), Shoji Ishibashi (National Institute of Advanced Industrial Science and Technology (AIST))

Gallium nitride is a direct wide-bandgap semiconductor and an ideal material for power electronics. In device structure fabrication, controlled impurity doping in a selective area is essential. Ion implantation is the most commonly used technique to control carrier concentrations. A drawback of ion implantation is the introduction of defects. Thus, controlling damage during and after ion implantation is a key for the reduction of residual defects in GaN. In the present study, we used monoenergetic positron beams constructed at University of Tsukuba and TUM FRM II to study the annealing behaviors of vacancy-type defects in Mg-implanted GaN.

Mg and H ions were implanted into GaN to obtain 0.1 and 0.7-micrometer-deep box profiles with Mg and H concentrations of 1E19 cm^{-3} and 2E20 cm^{-3}, respectively. For the as-implanted samples, the major defect species was determined to be Ga-vacancy related defects such as Ga-vacancy, divacancy, and their complexes with impurities. For Mg-implanted samples, an agglomeration of vacancies started at 800C annealing, leading to the formation of vacancy clusters. For Mg- and H-implanted samples, the hydrogenation of vacancy-type defects started after 800C annealing. Comparing with the annealing behavior of defects for the samples without H-implantation, the clustering of vacancy-type defects was suppressed, which can be attributed to the interaction between Mg, H, and vacancies.

Evolution of vacancies in thin film solar cells and in photochromic yttrium oxyhydride revealed by in-situ positron annihilation spectroscopy

Stephan Eijt (Delft University of Technology)

Tuesday, 13:40

Dibya Koushik (Eindhoven University of Technology), Frideriki Naziris (Delft University of Technology), Wenqin Shi (Delft University of Technology), Mirjam Theelen (Solliance Solar Research), Tom de Krom (Delft University of Technology), Diana Chaykina (Delft University of Technology), Henk Schut (Delft University of Technology), Werner Egger (Universität der Bundeswehr München), Marcel Dickmann (Universität der Bundeswehr München), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Adriana Creatore (Eindhoven University of Technology), Olindo Isabella (Delft University of Technology), Miro Zeman (Delft University of Technology), Bernard Dam (Delft University of Technology)

We apply Positron Annihilation Spectroscopy (PAS) to monitor the environmental degradation of ZnO/CIGS and perovskite thin film solar cells. Furthermore, yttrium oxy-hydride thin films are studied in view of their special photochromic properties, with the aim to elucidate the nature of vacancies in YOxHy and their evolution under in-situ UV illumination.

Our PALS study of as-deposited perovskite films using the PLEPS spectrometer reveals the presence of cation vacancies. Positron Doppler Broadening (DB-PAS) indicates that the degradation of MAPbI3 films involves the ingress of water molecules into the cation vacancies. In parallel, chemical transformations and a reduction in film thickness are observed, that proceed as a function of air exposure time.

PALS studies of ZnO:Al transparent electrode films on CIGS solar cells reveals a pronounced growth of vacancy clusters at the grain boundaries of the ZnO upon accelerated degradation at 85 oC/85% relative humidity. The growth of the vacancy clusters correlates with the observed degradation of the solar cell efficiency, pointing to a key role in the mechanism of degradation.

Finally, PALS reveals the presence of vacancies and micropores in photochromic YOxHy films. In-situ illumination DB-PAS studies show an increase in the S-parameter and a strong reduction in W, indicating that the generation of additional vacancies and/or a change in the charge state of vacancies accompanies the formation of the photochromic state.

The pulsed positron beams PLEPS and SPM for defect profiling with positron lifetime measurements at NEPOMUC: applications and developments

Werner Egger (Universität der Bundeswehr München)

Tuesday, 14:05

Gotfried Kögel (Universität der Bundeswehr München), Günther Dollinger (Universität der Bundeswehr München), Johannes Mitteneder (Universität der Bundeswehr München), Marcel Dickmann (Universität der Bundeswehr München), Peter Sperr (Universität der Bundeswehr München), Ricardo Helm (Universität der Bundeswehr München)

The pulsed low energy positron beam PLEPS is a user facility for defect-profiling with positron lifetime measurements using a monochromatic pulsed beam of variable implantation energy at the intense positron source NEPOMUC at the MLZ in Garching.

Typical applications of PLEPS comprise the defect identification in thin layers and layered structures of semiconductors and insulators, the investigation of irradiation induced defects in materials for fusion and fission as well as the characterization of open volumes in glasses, polymers, polymer- and membrane layers.

To investigate inhomogeneous defect distribution by positron annihilation lifetime spectroscopy a pulsed and focused positron beam is needed. For this purpose the Scanning Positron Microscope (SPM) was built and operated by the Universität der Bundeswehr München. To overcome the limitation of low count-rates obtainable with a laboratory source the SPM is currently transferred to the intense positron source NEPOMUC at the MLZ in Garching.
In this talk we will describe the present setup of PLEPS and its performance, and show some exemplary applications.Also, the setup of the SPM at NEPOMUC will be described. An outlook of future developments of PLEPS and SPM will be given.

click here to go to first page of this workshop

Positrons II

Tuesday – December 10th, 2019
15:00-16:30

15:00 - 15:15	**The Coincident Doppler-Broadening Spectrometer at NEPOMUC** *Vassily Vadimovitch Burwitz*
15:15 - 15:40	**Studies of thin film with NEPOMUC apparatuses: free volume and gas transport properties in biopolymers, defects in SiO_2, UO_2, ZnO oxides.** *Roberto Brusa*
15:40 - 16:05	**Results from Actual Studies using Pulsed Low Energy Positron Systems** *Vladimir Slugen*
16:05 - 16:30	**Positron-Electron Plasma – toward creation and study of a novel physical system using the NEPOMUC facility** *Matthew Stoneking*

The Coincident Doppler-Broadening Spectrometer at NEPOMUC

Vassily Vadimovitch Burwitz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Tuesday, 15:00

Leon Chryssos (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Lucian Mathes (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich),Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Thomas Schmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The capabilities of the Coincident Doppler-Broadening Spectrometer at the Neutron-induced Positron Source Munich (NEPOMUC) will be presented. In addition an overview of planned expansions will be given.

Two beam modes are available: standard operations provide a beam spot of >300 µm (FWHM) and micro beam for scanning with a reduced diameter of 33 µm (FWHM). Mearsurements may either be conducted as standard Doppler-broadening spectroscopy (DBS) where the signal at each detector is treated separately or in coincident Doppler-broadening mode (CDBS) where the detectors are run as coincidence pairs. CDBS provides a greatly improved signal to noise ratio (10^8) allowing the analysis of the chemical surrundings of defect. Currently four 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 T dependent defect spectroscopy, iii) a cryostat with T_{min}=40 K, iv) a device for in situ tensile tests. Ongoing improvement works include: an automated beam optimization system from which especially the micro beam mode will greatly profit. A planned increase in the number of detectors combined with an upgrade of the readout electronics, which should considerably reduce measurement times.

Studies of thin film with NEPOMUC apparatuses: free volume and gas transport properties in biopolymers, defects in SiO_2, UO_2, ZnO oxides.

Roberto Brusa (Department of Physics, University of Trento)

Tuesday, 15:15

I will review recent studies done thanks complementary and basic measurements carried out with NEPOMUC apparatuses. Depth resolved measurements with Positron annihilation lifetime spectroscopy (PALS), Doppler broadening spectroscopy (DBS) and coincidence Doppler broadening spectroscopy (CDBS) were performed in thin films.

Transport properties of light gas molecules were measured in biopolymer nanocomposite by gas permeation employing mass spectroscopy technique; gas barrier or sieve effects of cellulose nanofibrils, PHBH with dispersed graphene and PLA with dispersed cellulose were explained through the knowledge of the free volume structure as revealed by PALS. Defects induced by Ar and O ion implantation in ZnO were characterized by DBS and CDBS. Vacancy clusters formation and evolution in UO_2 as a function of annealing temperature and film deposition condition will be presented at the light of PALS, DBS and CDBS measurements; CDBS measurements were also compared with recent ab initio calculations.

Possible future experiments with improved apparatuses at NEPOMUC will be discussed.

click here to go to first page of this workshop

Results from Actual Studies using Pulsed Low Energy Positron Systems

Vladimir Slugen (Slovak University of Technology)

Tuesday, 15:40

Martin Petriska (Slovak University of Technology), Matus Saro (Slovak University of technolgy), Stanislav Sojak (Slovak University of Technology), Werner Egger (Universität der Bundeswehr München)

We are focused on the long term operation of nuclear reactors, which is one of the most discussed challenges in nuclear power engineering. The radiation degradation of nuclear materials limits the operational lifetime of all nuclear installations or at least decreases its safety margin. This paper is focused on experimental simulation and evaluation of materials via hydrogen ion implantation and comparison to our previous results obtained from neutron irradiated samples. The important results were obtained from the near surface studies using Pulsed Low Energy Positron System (PLEPS) in Garching. In our case, German reactor pressure vessel steels, originally from CARINA/CARISMA program, were studied by positron annihilation lifetime spectroscopy and pulsed low energy positron system with the aim to study microstructural changes in RPV steels after high level of irradiation. These results were compared to results from high level of hydrogen nuclei implantation. Defects with the size of about 1-2 vacancies with relatively small contribution (with intensity on the level of 20-40 %) were observed in all "as-received" steels. The increase in the size of the induced defects due to neutron damage was observed in the irradiated specimens resulting in 2-3 vacancies. On the other hand, the size and intensity of defects reached extremely high values due to displacement damage caused due to implantation of hydrogen ions in very narrow damaged region.

Positron-Electron Plasma – toward creation and study of a novel physical system using the NEPOMUC facility

Matthew Stoneking (Max-Planck-Institute for Plasma Physics)

Tuesday, 16:05

A Positron-Electron eXperiment (APEX) aims to produce magnetically confined, low temperature positron-electron plasma to test predictions that such a system with equal mass but oppositely charged species, in contrast to most laboratory and astrophysical plasma, is remarkably stable and exhibits other unique plasma characteristics. The magnetic trap will consist of a levitated superconducting coil (a=7.5 cm, I=30 kAt) that produces a dipolar magnetic field. To reach plasma conditions at a temperature of kT~5 eV, in the confinement volume of V≈15 liters, will require injection of between 10^{10} and 10^{11} positrons (and an equal number of electrons) into the trap (see talk by E.V. Stenson on plans to accumulate positrons from the NEPOMUC beam to create large pulses). In this talk, we will present results of experiments in a prototype trap that uses a supported permanent magnet (0.6 T at the pole surfaces). Positrons are successfully injected with nearly 100% efficiency into the dipole field using a combination of ExB drift, magnetic mirroring, and electrostatic reflection [1]. Once in the trap, some positrons orbits are confined for longer than 1 second, limited by transport associated with collisions with residual neutral gas molecules [2]. Plans for construction of the levitated dipole system at the NEPOMUC facility will also be presented.

[1] E. V. Stenson, et.al., Phys. Rev. Lett. 121, 235005 (2018).

[2] J. Horn-Stanja, et al., Phys. Rev. Lett. 121, 235003 (2018).

Positrons III

Tuesday – December 10th, 2019
17:00-18:00

17:00 - 17:15	**Upgrade of the NEPOMUC remoderator**	*Marcel Dickmann*
17:15 - 17:40	**Addition of a buffer-gas trap system to the NEPOMUC positron beam line**	*Eve Stenson*
17:40 - 18:00	**Summary**	

click here to go to first page of this workshop

Upgrade of the NEPOMUC remoderator

Marcel Dickmann (Universität der Bundeswehr München)

Tuesday, 15:40

Werner Egger (Universität der Bundeswehr München), Gotfried Kögel (Universität der Bundeswehr München), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Sebastian Vohburger (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Günther Dollinger (Universität der Bundeswehr München)

The neutron-induced positron source Munich (NEPOMUC) provides a monochromatic low-energy positron beam with an intensity of > $1 \cdot 10^9$ e^+/s and a diameter of ≈ 10 mm. To create a small beam focus or sharp positron pulses of 100 ps the beam brightness needs to be enhanced by re-moderation.

Based on the experiences with the remoderator setup, we redesigned and extended the existing construction. The new design allows a replacement of the remoderator crystal within several minutes and enables, therefore, a systematic test of different remoderator materials. Additionally, it is possible to clean and anneal the crystal surface by heating in-situ through electric current.

With the remoderator upgrade it was possible to increase the re-moderation efficiency and to raise both, the brightness and intensity of the beam. The effects of the higher beam quality have been already detected in positron annihilation lifetime spectra obtained with the Pulsed Low-Energy Positron System PLEPS. Here, the new setup leads to sharper pulses of ≤ 100 ps and a consequently better overall time resolution at a higher beam intensity. Moreover, from the increase of the brightness also other applications benefit, e.g. the Coincidence Doppler-broadening Spectrometer or the Scanning Positron Microscope, where an excellent phase space density of the beam is crucial to reach a high spatial resolution. The increased beam intensity will further reduce the measurement time of all instruments.

Addition of a buffer-gas trap system to the NEPOMUC positron beam line

Eve Stenson (Max-Planck-Institute for Plasma Physics, Technical University of Munich and University of California)

Tuesday, 16:05

J. R. Danielson (University of California), C. M. Surko (University of California), C. L. Manson (University of California), S. Ghosh (University of California), M. Dickmann (Universität der Bundeswehr München), Francesco Guatieri (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), S. Nißl (Max-Planck-Institute for Plasma Physics), A. Deller (Max-Planck-Institute for Plasma Physics), T. Sunn Pedersen (Max-Planck-Institute für Plasma Physics and Universität Greifswald), APEX Collaboration

The buffer-gas trap (BGT) is a well-established method for accumulating a steady-state stream of positrons into dense, cool, single-component clouds/plasmas, which can in turn be used to generate pulses or beams tailored to the application at hand [1]. BGTs are regularly employed in the creation of anti-atoms, the generation of positronium, studies of atomic and molecular interactions with antimatter, and a variety of surface and materials science techniques, just to name a few examples.

The e+ beams most commonly accumulated in BGTs come from Ne-moderated Na-22 and have a flux of <10^7 e+/s; this results in an upper limit on how many positrons can be accumulated and a lower limit on the time required to do so. The NEutron-induced POsitron source MUniCh (NEPOMUC) at FRM-II can deliver significantly more positron flux, up to 10^9 e+/s [2]. Preparations are underway to outfit NEPOMUC with a BGT system, after which an experimental program will determine the optimal combination of beam settings and trap settings for maximizing positrons/pulse. This will be a key step toward trapping enough positrons to create a magnetically confined plasma of half matter and half antimatter (a compelling frontier in plasma physics research and the goal of the APEX Collaboration) [3].

[1] J. R. Danielson, et al. Rev. Mod. Phys. 87, 247 (2015).

[2] C. Hugenschmidt, et al. New J. Phys. 14, 055027 (2012).

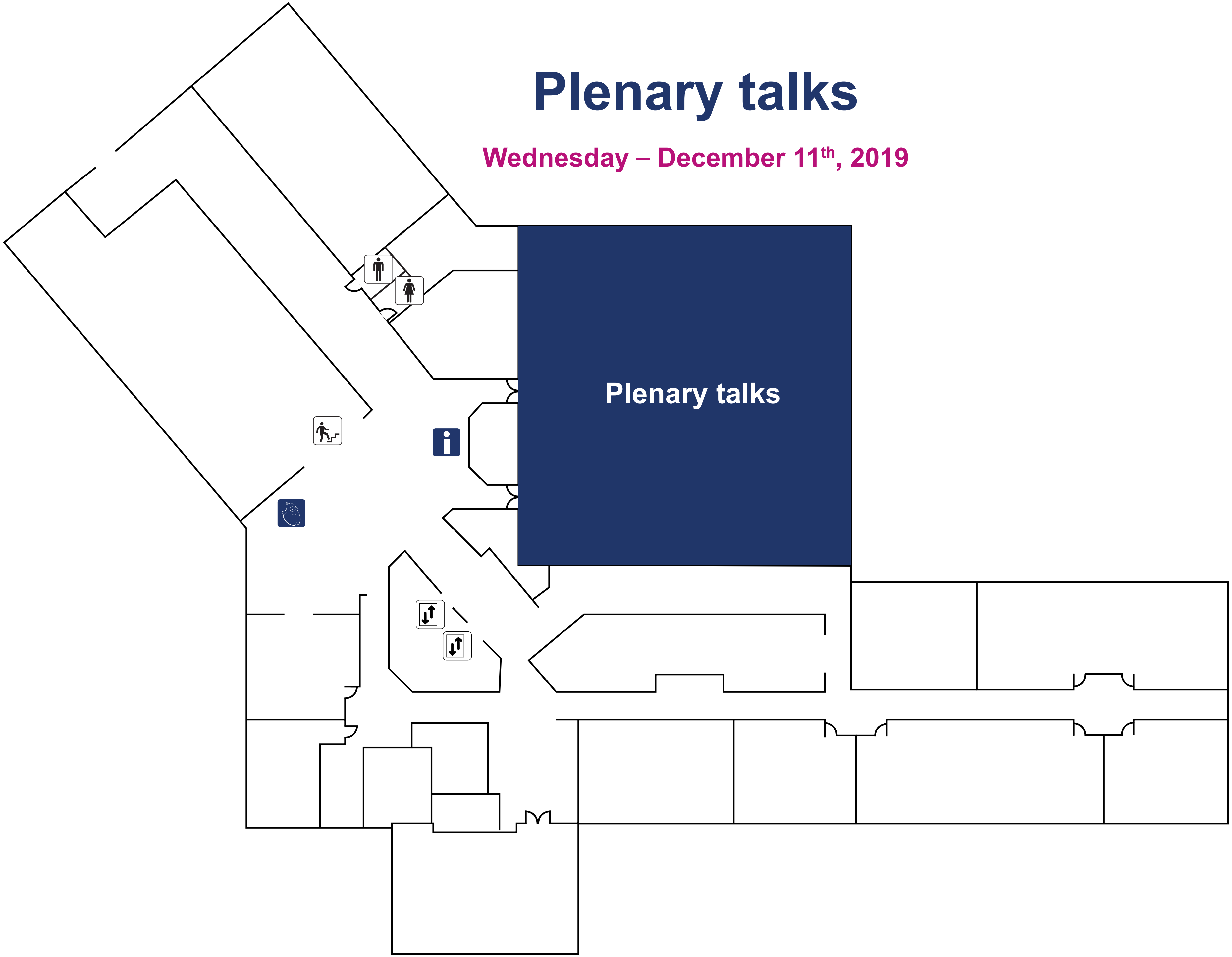
[3] T. Sunn Pedersen, et al. New J. Phys. 14, 035010 (2012).

WEDNESDAY

09:00	Welcome by the MLZ Directors	*Marriott Hotel Munich, Berliner Str. 93, 80805 München*
09:30 - 10:15	**Plenary Talk: Inner Structure and Dynamics of polymers at interfaces**	*Regine von Klitzing*
10:15 - 11:00	**Plenary Talk: Neutron Scattering Studies of Quantum Magnets**	*Bella Lake*
11:00	Coffee break	*Marriott Hotel Munich*
11:30 - 12:15	**Plenary Talk: Non destructive determination of the manufacturing methods of ancient Indian blades and modern replicas through advanced applications of neutron tomography and neutron diffraction**	*Francesco Grazzi*
12:15 - 12:30	**MLZ User Committee**	
12:30	Lunch	*Marriott Hotel Munich*
13:30	**Instrument control workshop**	
13:30	**Poster session**	

Plenary talks

Wednesday – December 11th, 2019



Plenary talks

Wednesday – December 11th, 2019
09:30-12:15

09:30 - 10:15	**Plenary Talk: Inner Structure and Dynamics of polymers at interfaces**	*Regine von Klitzing*
10:15 - 11:00	**Plenary Talk: Neutron Scattering Studies of Quantum Magnets**	*Bella Lake*
11:00	Coffee break	*Marriott Hotel Munich*
11:30 - 12:15	**Plenary Talk: Non destructive determination of the manufacturing methods of ancient Indian blades and modern replicas through advanced applications of neutron tomography and neutron diffraction**	*Francesco Grazzi*

click here to go to first page of this session

Inner Structure and Dynamics of polymers at interfaces

Regine von Klitzing (TU Darmstadt)

Wednesday, 09:30

Dikran Boyaciyan (TU Darmstadt), Matthias Kühnhammer (TU Darmstadt), Tetyana Kyrey (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH and Technische Universität Berlin), Judith Witte (Technische Universität Berlin), Olaf Holderer (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Stefan Wellert (Technische Universität Berlin)

The focus is on the inner structure and dynamics of polymers at solid and liquid interfaces studied by different neutron scattering techniques. For fabrication of stimuli responsive polymer coatings one challenge is to generate stable films which are still mobile and sensitive to outer parameters. The talk will address two different types of thin polymer films at interfaces: 1) films formed by deposition of hydrogel microgels and 2) by polymer brushes. During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest due to their thermoresponsive behaviour. Our work focuses on the effect of geometrical confinement on the phase volume transition and dynamics of these microgel particles at solid interfaces [1] and at liquid interfaces like in foams. The second example for stimuli sensitive coatings are polymer brushes (PNIPAM, PMETAC). They are doped with gold nanoparticles (AuNP) to make them sensitive to light or to changes in pH value. The correlation between the distribution of AuNP within the brush and the response of the AuNP/brush system to outer stimuli is of interest [2]. The dynamics of different polymer coatings were studied under grazing incidence (GISANS [3], GINSE [4]).

[1] S. Christau, et al. Polymer (2016) 98 454

[2] D. Boyaciyan et al., Soft Matter (2018) 14 4029

[3] S. Wellert, et al. Langmuir (2014) 30 7168

[4] K. Gawlitza, et al. Macromolecules (2015) 48 5807

Neutron Scattering Studies of Quantum Magnets

Bella Lake (Helmholtz Zentrum Berlin)

Wednesday, 10:15

Quantum magnetism studies the behaviour of magnetic materials where quantum fluctuations are strong and give rise to exotic behaviours not found in conventional magnets. It is possible to make model materials engineered for exhibit specific quantum. Of the experimental techniques available, neutron scattering has provided the deepest insights and most quantitative comparison to theory as will be illustrated by specific examples ranging from spin chains to frustrated magnets and spin liquids. New directions in this field will be outlined and the potential opportunities provided by new neutron instruments and sources.

Non destructive determination of the manufacturing methods of ancient Indian blades and modern replicas through advanced applications of neutron tomography and neutron diffraction

Francesco Grazzi (CNR-IFAC)

Wednesday, 11:30

Francesco Cantini (Opificio delle Pietre Dure), Davide Coco (Università di Roma la Sapienza), Floriana Salvemini (ANSTO), Burkhard Schillinger (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Anders Kaestner (Paul Scherrer Institut (PSI)), Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Antonella Scherillo (STFC - ISIS), Alan Williams (The Wallace Collection), David Edge (The Wallace Collection)

The analysis of the micro-structural features of ancient Indian blades has been carried out by neutron tomography and neutron diffraction. The results provide a clear identification of the different types of steel used to produce such weapons. Among them, only a small proportion of the large number of swords produced in India is made of hypereutectoid textured steel, namely wootz steel also known as “Damascus steel”. The others present characteristics very similar to the European swords produced in the same period.

The swords and daggers, provided by the Wallace Collection in London and the Bernisches Historisches Museum in Bern, as well as the modern replicas made by a professional swordsmith, were analyzed using neutron tomography both in white beam and energy selective configurations and neutron diffraction to get quantitative phase analysis and pole figure reconstruction of the texture in cementite phase. The results permitted to determine the spatial distribution of the iron and steel components inside the swords and the size and orientation of the microstructure of the ferrite and cementite grains in the wootz steel.

These results are an important starting point to lead to the comprehension of the metal preparation and the forging procedure to produce swords made of wootz steel. This kind of results is a further proof of the validity of the use of neutron techniques for non destructive and quantitative authentication and characterization of ancient metal artifacts.

Poster session

Wednesday – December 11th, 2019
14:00-16:30

Just click on the title to get directly to the abstract!

01	Jens Klenke	The experiment area MEPHISTO
02	Thomas Keller	High-resolution spectroscopy and diffraction at TRISP
03	Jügen Peters, Alexander Weber	Sample Environment at MLZ
04	Alexander Weber, Daniel Vujevic	Development in Sample Environment
05	Peter Link	The MLZ Neutron Optics Group
06	Marcell Wolf	TOFTOF cold neutron time-of-flight spectrometer at MLZ
07	Jitae Park	PUMA: thermal three-axes spectrometer equipped with multi-analyzer and unique polarization option
08	Manuel Scheel	In-situ GIWAXS measurements on 2-step slot-die printed thin-film perovskite layers for solar cell application
09	Wei Chen	Kinetics of Colloidal Quantum Dots during Printing
10	Igor Radelytskyi, Astrid Schneidewind	Panda a cold neutron TAS at MLZ
11	Weibo Hua	Determination of the structure of cobalt-free Li-Mn-rich oxides
12	Vladimir Hutanu	Dedicated neutron scattering instrument for complex magnetic structures POLI
13	Shanshan Yin	Nanostructured SnO_2 Templated by Amphiphilic Block Copolymer for Lithium-Ion Battery Anodes
14	Nicole Vorhauer	Visualization and quantification of freeze drying processes with neutron imaging
15	Markus Hoelzel	High Resolution Powder Diffractometer SPODI
16	Geethu Pathirassery Meledam	Investigations on the Growth Process of Poly(N-isopropylacrylamide) Mesoglobules under High-Pressure
17	Tobias Schrader, Andreas Ostermann	BIODIFF- Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum MLZ
18	Tobias Neuwirth	Targeted use of residual stresses in electric sheet to increase energy efficiency
19	Michael Schulz	The cold neutron imaging beam line ANTARES
20	Michael Schulz	A new high resolution detector system at ANTARES

21	Thomas Müller	DNS - diffuse neutron scattering spectrometer at MLZ
22	Bjørn Pedersen	RESI - The thermal single crystal diffractometer
23	Vitaliy Pipich	KWS-3 very small-angle neutron scattering focusing diffactometer at MLZ
24	Georg Glänzer	Interfaces in polymer based thin-film lithium-ion batteries
25	Nian Li	Highly ordered titania films with incorporated germanium nanoparticles calcined under different atmospheres
26	Xinyu Jiang	In-situ investigation of electrode sputter deposition for non-fullerene organic solar cell applications
27	Neelima Paul	Combining SANS with VSANS to extend q-range for morphology investigation of silicon-graphite anodes
28	Marie-Sousai Appavou	Cryo-TEM – A Complementary Technique for Neutron Scattering
29	Dominik Schwaiger	Studying the dynamics of PTB7:PCBM organic photovoltaic active layers
30	Josef Ketels	Future Upgrade of the 2D ACAR Spectrometer at NEPOMUC
31	Michael Hofmann, Weimin Gan	Materials Science Diffractometer STRESS-SPEC - Current status, new developments and future plans
32	Peixi Wang	Effect on Conformational Transformation of Methyl Side Group in Poly(sulfobetain)-Based Thermo-responsive Block Copolymer Thin Films
33	Suo Tu	Thermoelectric thin hybrid films based on PEDOT:PSS and inorganic nanoparticles
34	Alexander Hollering	Neutron optics for neutron beta decay studies with Proton Electron Radiation Channel (PERC)
35	Olaf Holderer	J-NSE “PHOENIX”: the neutron spin echo spectrometer upgrade at MLZ
36	Christoph Hugenschmidt	NEPOMUC – Positron Beam Facility and Instruments
37	Markus Trunk	Cold Neutron Depth Profiling at the PGAA facility
38	Chia-Hsin Ko	The Structural and Thermal Behavior of the Thermoresponsive Polymer Poly(N-isopropylmethacrylamide) in Aqueous Solution
39	Zsolt Revay, Christian Stieghorst, Xiaosong Li	Chemical analysis with Neutrons at the MLZ
40	Roy Schaffrinna	Thiophene based Semiconductors for Organic Solar Cells
41	Christian Weindl	Germanium-based nanostructure synthesis guided by amphiphilic diblock copolymer templating
42	Christian Franz, Johanna K. Jochum	The resonant neutron spin echo spectrometer RESEDA
43	Matthias Dodenhöft	Total Reflection High-Energy Positron Diffractometer at NEPOMUC
44	Gaetano Mangiapia	REFSANS: The horizontal time-of-flight reflectometer with GISANS option at the Heinz Maier-Leibnitz Zentrum
45	Weimin Gan	Lattice strain evolution of the solution heat-treated Mg-Ca alloys at room and elevated temperature under in-situ compressive deformation
46	Jia-Jhen Kang	Structural investigation on PTX-loaded poly(2-oxazoline) molecular brushes
47	Martin Meven	Diffraction Experiments under Extreme Conditions on Single Crystals with Hot Neutrons on HEiDi
48	Ralph Gilles	Materials Science group at Heinz Maier-Leibnitz Zentrum (MLZ)

49	Suzhe Liang	Highly-Regular Porous Germanium Oxide Thin Film Electrode for Lithium-ion Batteries
50	Xiaohu Li	Multi-scale phase quantification of strain-induced martensite in Austempered Ductile Iron (ADI) using different neutron diffraction techniques
51	Renjun Guo	What is the initial stage of degradation mechanism for perovskite solar cells?
52	Neslihan Aslan	QENS and in-situ SANS Investigations of Complex Hydrides
53	Wei Cao	Self-assembly of large magnetic nanoparticles in ultrahigh molecular weight linear diblock copolymer films
54	Kerstin Wienhold	In-situ printing of PBDB-T-SF:IT-4F for application in high-efficiency organic solar cells
55	Christina Geiger	Cononsolvency in PNIPAM-based block copolymer thin films
56	Sebastian Mühlbauer	Small-Angle Neutron Scattering Instrument SANS-1 at MLZ
57	Stefan Seidlmayer	Neutron & X-ray diffraction studies of graphite anodes conducted at MLZ
58	Daniel Steger	Influence of solvent on the morphology and optical properties of printed active layers based on PBDB-T-SF:IT-4F for application in organic solar cells
59	Julian Heger	Bio-hybrid thin films for templating titania nanostructures
60	Anna-Lena Öchsle	EMIM-DCA post-treatment of semi-conducting PEDOT:PSS polymer thin films to improve their thermoelectric properties
61	Simon J. Schaper	Revealing the formation of sputter deposited metal nanolayers on functional polymer thin films for lithium-ion batteries
62	Artem Feoktystov	KWS-1: High-flux SANS instrument with polarization analysis
63	Sebastian Grott	Printed organic thin films for photovoltaic applications – a morphology study
64	Heiko Trepka	Critical scattering in classical and quantum critical systems
65	Magdalini Spyranti	Synthesis of Mesoporous TiO_2 by using PS-b-P4VP as template block co-polymer: Fabrication and Analysis
66	Tianxiao Xiao	Wearable Electronic Skin based on Triboelectric and Luminescent Effect for Pressure and Tensile Sensing
67	Lu Qin	Studies on VDM alloy 780 Premium with standard heat treatments using synchrotron radiation
68	Frank Kümmel	Development of a new testing device for in-situ microstructural characterization under mechanical and thermal loading
69	Aurel Radulescu	KWS-2 - small angle neutron diffractometer
70	Tobias Widmann	3D printed humidity chamber for neutron scattering experiments
71	Johannes Mitteneder	Formation of a micrometer positron beam at the Scanning Positron Microscope
72	Dmitry Gorkov	KOMPASS – the polarized cold neutron triple-axis spectrometer at the FRM II
73	Alexandre Bertin	Bambus: a new inelastic neutron multiplexed analyzer for Panda at MLZ
74	Ting Tian	Morphology Tuning of ZnO Nanostructures for Hybrid Solar Cells
75	Linus Huber	Influence of printing temperature on the efficiency of organic solar cells
76	Michaela Zamponi	The high resolution neutron backscattering spectrometer SPHERES

77	Markus Singer	Simultaneous injection of positrons and electrons – progress towards a pair-plasma at NEPOMUC
78	Michael Heere	ErwiN in the making - a Fast Neutron Powder Diffraction Option
79	Daniel Sørensen	A New Measuring Cell for Operando Neutron Diffraction on Li-Ion Battery Cathode Materials
80	Cecilia Solis	In-situ characterization at high temperature of VDM alloy 780 Premium
81	Cecilia Solis	An innovative testing machine for heating, quenching, tension, compression and cracking studies of industrial relevant high-temperature alloys – HiMat BMBF project
82	Sabine Pütter	Free thin film sample preparation for Users by Molecular Beam Epitaxy
83	Julia Botinha	Characterization of VDM Alloy 718 CTP (DIN 2.4668 / UNS N07718) in different hardened conditions and the relationship between hardening phases and the alloy's hydrogen embrittlement susceptibility
84	Nicolas Walte	SAPHiR: Neutron diffraction and high resolution radiography under high pressure and temperature conditions
85	Daniel Hausmann	Optimising the γ/γ' microstructure and increasing the high temperature strength of a Co-base superalloy
86	Přemysl Beran	Phase transformations in CoRe-based alloys with Cr and Ni addition studied by in-situ neutron diffraction
87	Robert Georgii	The multi-purpose three-axis spectrometer (TAS) MIRA at FRM II
88	Ricardo Helm	Development of a new target station for external electric field application at PLEPS
89	Sandro Szabo	Self-diffusion in Mercury investigated with quasi-elastic neutron scattering
90	Dominik Petz	Non-uniform capacity fading in lithium-ion batteries revealed by spatially-resolved diffraction of neutrons and synchrotron radiation
91	Stefan Strangmüller	Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate $Li_{14}SiP_6$
92	Jiangong Zhu	Investigation of capacity fade mechanisms and modeling for lithium ion batteries cycled under different state of charge ranges
93	Kiril Krezhov	On the use of $BaCe_{0.85}Y_{0.15}O_{3-d}$ as a multi-functional ingredient in solid oxide fuel cells
94	Mathias Bersweiler	Size-dependent spatial magnetization profile of Manganese-Zinc ferrite nanoparticles
95	Yury Khaydukov	NREX – polarized neutron/X-ray reflectometer
96	Jens Krueger	NICOS - The instrument control user interface
97	Adrian Losko	Combined Neutron and Gamma Tomography at the NECTAR instrument
98	Yannick Meinerzhagen	POWTEX – Angular- and Wavelength Dispersive, High-Intensity Neutron TOF Diffractometer
99	Vassily Vadimovitch Burwitz, Leon Chryssos, Lucian Mathes, Thomas Schmidt	The Coincident Doppler-Broadening Spectrometer at NEPOMUC
100	Apostolos Vagias	Monitoring selectivity of gold cluster growth/formation on antifouling-relevant zwitterionic thin block copolymer coatings

click here to go to the poster list

1

The experiment area MEPHISTO

Jens Klenke (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The MEPHISTO experimental area is prepared for hosting the new PERC experiment. The actual status of the experimental area will be reported. There will also be an outlook for the technical infrastructure which is in advanced planning status.

2

High-resolution spectroscopy and diffraction at TRISP

Thomas Keller (Max Planck Institute for Solid State Research)

Matthias Hepting (Max Planck Institute for Solid State Research), Heiko Trepka (Max Planck Institute for Solid State Research), Franz Tralmer (Max Planck Institute for Solid State Research), Bernhard Keimer (Max Planck Institute for Solid State Research)

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 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.

3

Sample Environment at MLZ

Jürgen Peters (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)
Alexander Weber (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Beside state of the art neutron scattering instrumentation, sample environment is an important pillar to attract the user community. For the efficient use of neutrons, close collaboration between users, instrument scientists and sample environment team is particularly important in order to run experiments smoothly or to provide sample environment for current and future requirements. Some new available devices and developments are presented like new available magnet or high temperature furnaces enabeling gasflow and quench options. The user meeting is very convenient for interchange and discussion amongst users and central groups to initiate new developments.

4

Development in Sample Environment

Alexander Weber (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)
Daniel Vujevic (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

We will present our newest developments in sample environment equipment together with our freshly bought racing horses. This will cover magnets, cryostats, fluids and humidity.

click here to go to the poster list

5

The MLZ Neutron Optics Group

Peter Link (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Sergey Masalovich (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

We present our state of the art neutron guide production and other service for the instruments. This comprises also the usage of ^{3}He filter cells for neutron polarisation.

6

TOFTOF cold neutron time-of-flight spectrometer at MLZ

Marcell Wolf (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Wiebke Lohstroh (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Marcell Wolf (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Zachary Evenson (Springer Heidelberg)

TOFTOF is a direct geometry disc-chopper time-of-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 ^{3}He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 12 m^2 (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.

7

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

Jitae Park (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Avishek Maity (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Juergen Neuhaus (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Götz Eckold (Georg-August University of Göttingen)

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.

8

In-situ GIWAXS measurements on 2-step slot-die printed thin-film perovskite layers for solar cell application

Manuel Scheel (Department of Physics, Technical University of Munich)

Lennart Reb (Department of Physics, Technical University of Munich). Sebastian Grott (Department of Physics, Technical University of Munich), Renjun Guo (Department of Physics, Technical University of Munich), Matthias Schwartzkopf (DESY), Stephan Roth (DESY / KTH), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Reaching minimodule efficiencies of around 17% in 2018 and 15% on ultrathin flexible substrates, commerzialisation of thin-film organic-inorganic metal halide perovskite based solar cells (PSCs) is very promising as next generation solar cells. However, further improvement on upscaling is needed to push for commercializiation. In principle, industrial requirements for fabrication can be met by roll-to-roll slot-die coating. In-situ GIXS measurements are well suited for kinetic studies and deliver stochastically relevant information from a relatively large sample area. In-situ GIWAXS measurements were performed on 2-step deposited methyl ammonium lead iodide (MAPI) films during the annealing process. Slot-die printed samples were compared with spin coated samples. MAPI thin films were prepared on glass coated with ITO and PEDOT:PSS. Annealing kinetics, changes in crystal structure and crystal orientation of printed thin films were analyzed and compared to spincoated samples.

9

Kinetics of Colloidal Quantum Dots during Printing

Wei Chen (Department of Physics, Technical University of Munich)

Haodong Tang (Southern University of Science and Technology), Nian Li (Department of Physics, Technical University of Munich), Manuel Scheel (Department of Physics, Technical University of Munich), Volker Körstgens (Department of Physics, Technical University of Munich), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron (DESY)), Stephan Roth (Department of Electrical and Electronic Engineering), Kai Wang (Southern University of Science and Technology), Xiao Wei Sun (Southern University of Science and Technology), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Colloidal quantum dots (QDs) are considered as a promising candidate for being used in next-generation solution-processed thin-film optoelectronic applications. The presently investigated QD thin films are mainly fabricated by a spin-coating, which is a lab-scaled (small-scaled) deposition method and the insights from the structure related aspects are supposed to be limited in a large scalable deposition method, like printing. In current work, we used real-time grazing-incidence small-angle X-ray scattering (GISAXS) to observe the QD kinetics during printing. The 2D GISAXS patterns indicate that QDs have formed an apparent well-ordered layer during the film's wet-dry transition. The layer acts a templating layer for the further particle stacking and the final film-forming. The inter-distance of QDs and the stacking behavior are further analyzed with a superlattice configuration.

10

Panda a cold neutron TAS at MLZ

Igor Radelytskyi (Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany)
Astrid Schneidewind (Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany)

Alexandre Bertin (Institut für Festkörperphysik, Technical University Dresden)

Investigations of magnetic excitations focus on new magnetic materials, quantum magnetism, superconductivity, heavy-fermion or low-dimensional systems, frustrated and multiferroic materials. The challenges of high-resolution studies can be answered only by cold neutron (TAS) spectroscopy experiments.

In our days, there is a trend for extreme conditions, searching for exotic spin states. The discovery of these systems is often limited by small sample sizes or weak scattering cross sections, as well as asking for special sample environment such as high magnetic fields and low temperatures. PANDA, being a high-resolution, high-flux cold neutron TAS spectrometer with a remarkably low background, successfully contributes with high-level experiments to a broad variety of scientific topics.

We will report here about the successfully performed and published user experiments on systems mentioned above where PANDA significantly contributed.

click here to go to the poster list

11

Determination of the structure of cobalt-free Li-Mn-rich oxides

Weibo Hua (Karlsruhe Institute of Technology (KIT))

Björn Schwarz (Karlsruher Institute of Technology (KIT)), Michael Knapp (Karlsruher Institute of Technology (KIT)), Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Joachim R. Binder (Karlsruhe Institute of Technology (Karlsruher Institute of Technology (KIT)), Sylvio Indris (Karlsruhe Institute of Technology (Karlsruher Institute of Technology (KIT)), Helmut Ehrenberg (Karlsruher Institute of Technology (KIT))

Cobalt-free lithium- and manganese-rich layered oxides ($Li[Li_xNi_yMn_{1-x-y}]O_2$, LMLOs) has catalyzed intensive research efforts to determine their structure that could accommodate a relatively large amount of lithium ions. This feature can make the LMLO electrodes more competitive than the conventional $Li[Ni_xCo_yMn_{1-x-y}]O_2$ (NCM) cathodes for Li-ion batteries. However, whether LMLOs should be regarded as accumulation of layered monoclinic phase (C2/m) and layered rhombohedral phase (R-3m) nanodomains or as a layered monoclinic single-phase solid solution (C2/m) remains an open question. Herein, high-resolution neutron powder diffraction at the instrument SPODI was used to investigate the localisation and quantification of lithium and oxygen in the structure. Combined with the analysis of synchrotron radiation diffraction and electron diffraction, we demonstrate that the structure of $Li[Li_{0.2}Ni_{0.2}Mn_{0.6}]O_2$ is a single monoclinic solid solution layered structure with ultrathin spinel/rock-salt-type surface. These results contribute to a profound analysis of the relationship between electrochemical performances and the structure of LMLOs.

12

Dedicated neutron scattering instrument for complex magnetic structures POLI

Vladimir Hutanu (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ)

Hao Deng (RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Polarized single-crystal diffractometer POLI at MLZ employs non-polarized double-focusing monochromators in combination with high-efficiency ^{3}He cell polarizers, which lead to a gain in both flux and resolution in comparison with other short-wavelength polarized neutron diffractometers using Heusler-alloy monochromators. With flexible instrument setups, namely: 1) classical single crystal neutron diffraction in extreme environments like high magnetic fields, very low/high temperatures, high voltage, pressure cells etc. and their combinations; 2) polarize neutron diffraction (flipping-ratio measurements) using high magnetic field and 3) zero-field spherical neutron polarimetry using the third generation Cryopad, and rather high flux of hot polarized neutron, POLI raises to a powerful tool in complex magnetic structure research. Recently 8 T magnet for magnetic phase diagrams and polarized diffraction has been implemented on POLI. Typical applications of the instrument are: 1) basic magnetic structure refinement, 2) magnetic structure studies under very low temperature and high pressure, 3) distinguish between magnetic spin density wave, helicoidal or cycloidal chiral structures, 4) separate incommensurate structures with very long period, 5) magnetic domain study with depolarization analysis. Our versatile instrument gives a unique access to understanding complicated magnetic structures and offers a good starting point for further exploring dynamics in novel magnetic physics.

13

Nanostructured SnO_2 Templated by Amphiphilic Block Copolymer for Lithium-Ion Battery Anodes

Shanshan Yin (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

With the rapid development of wireless information communication products, electric vehicles, power tools and other fields, higher requirements are placed on the energy density, power density and lifetime of lithium-ion batteries. Compared with conventional graphite anodes, SnO_2 afforded much higher theoretical specific capacity (1494 $mAhg^{-1}$). However, the big volume change and the continuously generated SEI film during the cycling leads to a serious capacity recession, which therefore limits its practical application. In the present work, a novel mesoporous SnO_2 anode has been was successfully synthesized by an amphiphilic block copolymer assisted sol-gel process, which is expected to facilitate the infiltration of the electrolyte and accommodate the volume expansion of the material during cycling, thereby improving the electrochemical performance of the electrode. The pore arrangement of the obtained SnO_2 nanostructure is studied via scanning electron microscopy (SEM) and grazing-incidence small-angle X-ray scattering (GISAXS).

14

Visualization and quantification of freeze drying processes with neutron imaging

Nicole Vorhauer (Otto-von-Guericke-Universität Magdeburg)

Petra Först (School of Life Sciences Weihenstephan, Technical University of Munich)

Neutron radiography and tomography are very efficient imaging techniques that allow visualization and study in-situ the kinetics and major effects of primary freeze-drying. The methods complement the classical measurement techniques in freeze-drying that only indirectly obtain the relevant information based on the measurement of usually pressure and temperature. The main advantage of neutron imaging is the possibility to observe the drying process in-situ in a fully equipped set-up; this has never been presented before. It allows accurate track of the position of the sublimation front which is not possible with the classical tools. Based on this we could study for the first time the dependence of the local velocity of the sublimation front on the drying conditions. For example, we were able to visualize that the structure of the sublimation front basically depends on the particle size of the freeze drying product. Further experiments for a systematic study of the interrelation of particle size, solid content and drying conditions are already in preparation. They are necessary to identify the limits of freeze-drying regimes that depend on the process conditions. In the user meeting we will present the results from measurements at FRM II and at PSI (Villigen/Switzerland). We will highlight the major outcomes and discuss the modifications required for future measurements.

15

High Resolution Powder Diffractometer SPODI

Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Helmut Ehrenberg (Karlsruher Institute of Technology (KIT)), Josef Pfanzelt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Volodymyr Baran (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

16

Investigations on the Growth Process of Poly(N-isopropylacrylamide) Mesoglobules under High-Pressure

Geethu Pathirassery Meledam (Department of Physics, Technical University of Munich)

Marie-Sousai APPAVOU (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Bart-Jan Niebuur (Department of Physics, Technical University of Munich), Christine Papadakis (Department of Physics, Technical University of Munich), Vitaliy Pipich (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Alfons Schulte (University of Central Florida)

Poly(N-isopropylacrylamide) (PNIPAM) in aqueous solution forms stable dispersions of mesoglobules upon heating through the cloud point. At atmospheric pressure these mesoglobules are small and strongly dehydrated, and their further growth and coalescence are hindered by the viscoelastic effect. On the contrary, at high pressures, larger clusters of PNIPAM mesoglobules are formed, which are more hydrated. Here, we investigate the growth process of PNIPAM mesoglobules upon increasing and decreasing pressure using very small angle neutron scattering (VSANS) at KWS-3, FRM II. As pressure is increased, the size of the mesoglobules increases markedly at a critical pressure, which is found to depend on temperature. Upon decreasing pressure below the critical pressure, two populations of mesoglobules having sizes of the order of smaller mesoglobules and larger clusters are observed. We conjecture that the strong influence of pressure on the growth process of PNIPAM mesoglobules is due to the pressure-dependent hydration and subsequent aggregation of mesoglobules.

17

BIODIFF - Macromolecular Neutron Diffraction at the MLZ

**Tobias Schrader (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)
Andreas Ostermann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)**

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 FRM II 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.

18

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

Tobias Neuwirth (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich

Ines Moll (Department of Mechanical Engineering (utg), Technical University of Munich), Benedikt Schauerte (RWTH Aachen), Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Peter Böni (Department of Physics, Technical University of Munich)

Electrical steel sheets are used in electric drives to guide the magnetic field. The efficiency of an electrical steel sheet strongly depends on the amount of energy lost during the reversal of magnetization, which is dependent on the mobility of the magnetic domains. The mobility of the magnetic domains is influenced by stress caused during the manufacturing process. [1],[2].

To probe the magnetic domain constellation in bulk samples of technically relevant dimensions neutron grating interferometry (nGI) is the technique of choice, as it allows to probe the bulk local magnetic properties, which is not possible with most other techniques.

nGI provides information about the amount of ultra-small-angle-neutron scattering inside a sample [3]. The resulting image (DFI) is sensitive to the distribution of magnetic domain walls, which serve as possible scattering centers. Hence the DFI signal is related to the distribution and size of magnetic domains inside a sample, allowing 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.

This project is done together with the utg (TUM) and IEM (RWTH Aachen) as part of the DFG priority programm SPP2013 .

[1] H. Weiss et al., pending (2018)

[2] A. Moses, IEEE Trans. Magn, Vol. 15, 1575-1579 (1979)

[3] C. Grünzweig, PhD thesis (2009)

19

The cold neutron imaging beam line ANTARES

Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Burkhard Schillinger (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Alexander Backs (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Dominik Bausenwein (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Peter Böni (Department of Physics, Technical University of Munich), Tobias Neuwirth (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Marc Seifert (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

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.

20

A new high resolution detector system at ANTARES

Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Jacot-Guillarmod Mathieu (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Yiyong Han (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Severin Vierrath (IMTEK, Universität Freiburg), Mathias Breitwieser (IMTEK, Universität Freiburg)

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 resoution 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.

DNS – diffuse neutron scattering spectrometer at MLZ

21

Thomas Müller (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Yixi Su (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

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).

RESI – The thermal single crystal diffractometer

22

Bjørn Pedersen (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

RESI is the single crystal diffractometer for medium-sized and complex structures wiht thermal neutrons.

The diffractometer RESI is designed for high q-resolution, low background and best flux usage allowing optimum measurements of weak diffraction phenomena in a large portion of the reciprocal space on single crystalline samples.

- Structure analysis, bonding theory, electron densities: Due to the interaction with atomic cores and the diffraction angle independence of the atomic form factor, it is possible to measure Bragg scattering up to high diffraction angles.
- Real crystals and compounds of interest for material science are often not perfectly ordered. The elucidation of these real structures requires the analysis of the corresponding diffuse scattering. The diffuse scattering – off the Bragg reflections – is normally differentially weak and distributed continually (anisotropic) in the reciprocal space.
- Modulated structures show satellite reflections at “incommensurable” positions. Both areas require analysis of large portions of the reciprocal space.
- Twinned crystals and multi-domain/multi-phase crystals are often difficult to measure on single-counter instruments. The area detector at RESI allows for easy detection and in many cases separation of reflections in such systems.

23

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

Vitaly Pipich (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Baohu Wu (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

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 $3 \cdot 10^{-5}$ and $2 \cdot 10^{-2}$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 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°C to 140°C), high-temperature furnace (<1900°C), cryostats/inserts (>20mK), liquid pressure cell (<5kBar/10-80°C), CO_2/CD_4 gas pressure cell (<0.5kBar/10-80°C), humidity cell/generator (5-95%/10-90°C), magnets (horizontal <3T, vertical <2.2T), Bio-logic® multimixer stopped flow (5-80°C), rheometer RSA II (tangential/radial) etc.

24

Interfaces in polymer based thin-film lithium-ion batteries

Georg Glänzer (Department of Physics, Technical University of Munich)

Simon Schaper (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

With rising importance of renewable energy sources the need for reliable energy storage-solutions grows. Most batteries used currently in industry are lithium-ion batteries (LIBs) with liquid electrolytes. Due to the inflammable nature of liquid electrolytes LIBs are prone to dangerous damage preventable by solid state electrolytes based on polymers. However the ionic conductivity still needs to be increased. Polyethylene oxide (PEO) is a well known Li-ion conducting polymer. Its shortcomings in terms of physical stability can be compensated by using block copolymer electrolytes (BCEs). Changing the block length or the solvent environment preparing thin films can be used to manipulate the morphology of the BCE system. Polystyrene-block-polyethylene oxide (PS-b-PEO) has been investigated extensively as electrolyte. The PS block offers mechanical stability while the PEO part is able to solvate lithium ions. Adding the lithium salt lithium bistrifluoromethanesulfonimidate (LiTFSI) provides the necessary lithium-ions as charge carriers for the electrolyte. Thin-film batteries are built using this polymer electrolyte. In-operando SAXS measurements provide insight into changes in the polymer's morphology. The contrast between the two polymer blocks, caused by different electron densities, allows for an analysis of the electrolyte's structural evolution by nondestructive scattering experiments. Previous works have already shown the importance of in-operando measurements.

25

Highly ordered titania films with incorporated germanium nanoparticles calcined under different atmospheres

Nian Li (Department of Physics, Technical University of Munich)

Yin Shanshan (Department of Physics, Technical University of Munich), Julian Heger (Department of Physics, Technical University of Munich), Roy Schaffrinna (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Mesoporous titania films with ordered nanostructures show great promise in various applications, such as solar cells. To optimize solar cell performance, pre-synthesized crystalline germanium nanoparticles around 10 nm are introduced into mesoporous titania films. The influence of different calcination atmospheres (air and argon) on the morphology and properties of TiO_2/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 TiO_2/Ge composite films calcined in air and argon 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 calcination under different atmospheres, the optimized morphology and properties of TiO_2/Ge composite films will be obtained, providing a promising candidate for solar cell photoanodes.

26

In-situ investigation of electrode sputter deposition for non-fullerene organic solar cell applications

Xinyu Jiang (Department of Physics, Technical University of Munich)

Simon Jakob (Technical Unniversity of Munich), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron DESY), Stephan V. Roth (Deutsches Elektronen-Synchrotron DESY), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Recently, the efficiencies of non-fullerene organic solar cells (OSCs) with small molecule acceptors rapidly increased to over 16%, which makes OSCs competitive to commercial available solid state solar cells. Except for the active layer, OSC performance is strongly influenced by the quality of anode layer, since it offers a path for carriers transport. Therefore understanding how metal electrodes grow on the active layer as well as the blocking layer plays a significant role in achieving high efficiency solar cells. For understanding the mechanism of the metal cluster growth on the active layer with various morphology, we introduce in-situ grazing incidence small angle X-ray scattering (GISAXS) technique to observe the morphology change during anode sputtering process. In addition, atomic force microscopy (AFM) and scanning electron microscope (SEM) techniques were used to get the surface morphology information of sputtered layers.Previous works have already shown the importance of in-operando measurements.

click here to go to the poster list

27

Combining SANS with VSANS to extend q-range for morphology investigation of silicon-graphite anodes

Neelima Paul (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Henrich Frielinghaus (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Vitaliy Pipich (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Silicon-based electrodes are attractive candidates as anodes for Li-ion batteries due to their high theoretical specific capacity. However, repeated lithiation/delithiation causes significant morphological changes of the silicon particles which results in formation of highly porous silicon structures and severe side reactions at the silicon/electrolyte interface. To quantify such morphological changes in the micrometer as well as on the nanometer scale, we combine very small-angle neutron scattering (VSANS) and small-angle neutron scattering (SANS) techniques. While conventional and contrast-matched SANS data provide insights into the solid-electrolyte-interphase (SEI) coverage around the silicon particles and filling of the evolving porosity within the electrode, VSANS data provide information on the micrometer-sized graphite particles.

28

Cryo-TEM – A Complementary Technique for Neutron Scattering

Marie-Sousai APPAVOU (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

The neutron instrumentation at the MLZ, in particular Small Angle Neutron Scattering, reflectometry and macromolecular crystallography allow to investigate structures in the range from 1 nm up to several hundred nm in reciprocal space. In soft matter and biology the 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; virtually it may complete and enhance any SANS investigation on soft matter investigation.
A transmission electron microscope (TEM) is available at the Jülich Center for Neutron Sciences at MLZ in the JCNS building.
The instrument is a 200 kV JEM-FS2200 from JEOL with a field emission gun (FEG) and an on-line Omega Energy Filter allowing measurements at magnification from x 50 to x 1 M with a resolution of 0,2 nm in point and 0,1 nm in lattice. The Microscope is equipped with a Tietz CMOS camera with 2048 x 2048 pixels square area. The soft matter thin samples (max- ~100nm) have to be investigated either in dried or frozen state (Cryo-TEM) to be able to work in the necessary vacuum and to suppress blurring motion of the object as well as radiation damage. The TEM laboratory comprises an extended suite of preparation equipment. Users will be supported by JCNS scientists (M.S. Appavou) to conduct the suitable preparation and TEM investigation.

29

Studying the dynamics of PTB_7:PCBM organic photovoltaic active layers

Dominik Schwaiger (Department of Physics, Technical University of Munich)

Wiebke Lohstroh (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active materials due to their superior performance compared to e.g. planar layered 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 [1].
A frequently applied and well-studied system is the combination of P3HT ($(C_{10}H_{14}S)n$) as electron donor and PCBM ($C_{72}H_{14}O_2$) 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 [2], [3]. A novel, very promising electron donor material is PTB7 ($(C_{41}H_{53}FO_4S_4)n$). We produced films of PTB7, PCBM and a mixture of these two from a chlorobenzene solution and performed first quasielastic neutron scattering (QENS) experiments on this system in order to evaluate the dynamics of pure compounds as well as blend films on a pico- to nanosecond timescale and potential influences of manufacturing parameters (e.g. mixing ratio, solvent choice, annealing time/temperature). QENS experiments were performed at the MLZ instrument TOFTOF in a temperature range between 150 K and 400 K.

[1] H. Wang et al. (2014), Materials, 7, 2411–2439

[2] A. Guilbert et al. (2016), The Journal of Physical Chemistry Letters, 7, 2252–2257

[3] T. Etampawala et al. (2015), Polymer, 61, 155–162

30

Future Upgrade of the 2D ACAR Spectrometer at NEPOMUC

Josef Ketels (Department of Physics, Technical University of Munich)

Two dimensional angular correlation of annihilation radiation (2D ACAR) is a powerful probe for the investigation of the electronic structure of materials. In ACAR a 2D projection of the two-photon momentum density is recorded, which is closely related to the electron momentum density. From a series of such measurement at different projection angles the 3D Fermi surface(s) can be reconstructed. The current ACAR spectrometer at the Technical University Munich uses positrons from a ^{22}Na source, which enables spin-resolved measurements of the bulk electronic structure. Various questions that have been successfully tackled at our spectrometer are the reconstruction of the spin-resolved Fermi sheets of Cu_2MnAl [1], the electron-electron correlation strength in nickel [2] or the electronic correlations in vanadium [3].
In a future upgrade the spectrometer will be moved to the positron beamline at the NEPOMUC positron source of FRM II. The utilization of the mono-energetic positron beam allow the depth resolved investigation of the electronic structure. This opens the possibility to clarify questions on the evolution of the electronic structure from surface to bulk and to measure layered systems.

[1] J.A. Weber, et al., PRL 115 (2015) 206404

[2] H. Ceeh, et al., Sci. Rep. 6 (2016) 20898

[3] J.A. Weber, et al., PRB 95 (2017) 075119

click here to go to the poster list

31

Materials Science Diffractometer STRESS-SPEC - Current status, new developments and future plans

Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)
Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Joana Rebelo-Kornmeier (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Xiaohu Li (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Markus Lieret (Friedrich-Alexander Universität Erlangen-Nürnberg (FAU)), Heinz-Günter Brokmeier (TU Clausthal)

STRESS-SPEC is the dedicated diffractometer for materials science applications at MLZ. It offers high thermal neutron flux and is mainly used for fast residual strain and texture (bulk, local or gradient) measurements [1, 2]. Recent upgrades include a new detector system developed in-house, a new fully automatic slit system for gauge volume definition of the monochromatic beam, and a quenching / deformation neutron dilatometer. As a further development and in line with the new slit system we developed a new radial collimator to shape the gauge dimensions of the monochromatic beam impinging on the sample. Here we will present results of the commissioning experiments of the collimator together with giving an overview of the current capabilities of the diffractometer.
STRESS-SPEC has pioneered the use of robotic sample manipulation [2, 3] and improvements of the position accuracy of this device through a new adaptive control system will be outlined as well.

[1] M. Hofmann et al, Mater. Sci. Forum. 524-525, 211-216 (2006)

[2] H.-G. Brokmeier et al, Nucl. Inst. & Meth. in Phy. Res. A 642, 87-92 (2011)

[3] C.R. Randau et al, Nucl. Inst. & Meth. in Phy. Res. A 794, 67-75 (2015)

32

Effect on Conformational Transformation of Methyl Side Group in Poly(sulfobetain)-Based Thermo-responsive Block Copolymer Thin Films

Peixi Wang (Department of Physics, Technical University of Munich)

Lucas P. Kreuzer (Department of Physics, Technical University of Munich), Christina Geiger (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Classic zwitterionic poly(sulfobetaine)s, poly(4-((3-methacrylamidopropyl)dimethyllammonio) butane-1-sulfonate)) (PSBP), which exhibit an upper critical solution temperature (UCST) in aqueous media, have been widely used to investigate its swelling/deswelling behavior and phase transition mechanism. Also its block copolymers reached high attention if they contain other broadly studied nonionic thermo-responsive polymers, especially poly(N-isopropylacrylamide) (PNIPAM) and poly(isopropylmethacrylamide)(PNIPMAM), which feature a lower critical solution temperature (LCST) in aqueous solution, normally higher than UCST of PSBP. However, a comparison between the block copolymer films of PSBP-b-PNIPAM and PSBP-b-PNIPMAM, with a similar degree of polymerization and thickness of film, is still missing. We present a comparison of the humidity- induced swelling/deswelling behavior of block copolymer thin films of PSBP-b-PNIPAM and PSBP-b-PNIPMAM with a similar degree of polymerization and thickness in aqueous vapor atmosphere as studied by time-of-flight neutron reflectometry (TOF-NR). Ellipsometer results, when adjusting the spin coating parameters, contributed to control the thickness to 50-60 nm. The resulting polymer films were also characterized by Fourier transform infrared (FTIR) spectroscopy.

click here to go to the poster list

33

Thermoelectric thin hybrid films based on PEDOT:PSS and inorganic nanoparticles

Suo Tu (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

PEDOT:PSS is the most studied conducting polymer system owing to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric devices. 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. However, it is difficult to obtain a high ZT value, owing to the fact that the parameters S, σ, and k are interdependence as a function of carrier concentration and hard to be optimized simultaneously. To date, there are two promising approaches to significantly enhance ZT values of PEDOT:PSS. One is doping organic solvents. Another effective way to enhance the TE performance of PEDOT:PSS is to introduce inorganic nanomaterials with high TE property into conducting polymer matrix. Here, PEDOT:PSS thin films are nanostructured with inorganic nanoparticles and doped with organic solvents in order to optimize their TE performance. The surface and inner morphology are probed using scanning electron microscopy, atomic force microscopy and grazing-incidence wide/small-angle X-ray scattering, respectively. Additionally, UV-Vis spectroscopy, Raman spectroscopy and X-ray photoelectron spectroscopy are employed to investigate the mechanism behind for TE performance improvement.

34

Neutron optics for neutron beta decay studies with Proton Electron Radiation Channel (PERC)

Alexander Hollering (Department of Physics, Technical University of Munich)

Bastian Märkisch (Department of Physics, Technical University of Munich), Thorsten Lauer (Movatec GmbH) Ulrich Schmidt (Universität Heidelberg)

The PERC experiment is currently under construction at the new beam port MEPHISTO at the FRMII. 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}.
The author will present an overview of the demanding experimental constraints for this precision experiment, concerning the beamline with its' neutron optical components. In the framework of this experiment, the author will present the current status of the development of a completely non-depolarizing supermirror coating from Copper/Titanium. First tests were made in 2014 by N.Rebrova in the scope of her PhD-thesis. Based on the work of A. K. Petukhov et. al., the author will also present the results for a solid-state neutron polarizer made from Iron/ Silicon coating.

click here to go to the poster list

35

J-NSE "PHOENIX": the neutron spin echo spectrometer upgrade at MLZ

Olaf Holderer (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Stefano Pasini (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Tadeusz Kozielewski (Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH), Michael Monkenbusch (Jülich Centre for Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH)

Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. In 2017 the Jülich neutron spin echo at MLZ went through a refurbishment of the secondary spectrometer: The old normal conducting main-precession coils have been replaced by a new set of fringe-field compensated, superconducting magnets that were realized following the results obtained for the design of ESSENSE, the proposed high-resolution NSE spectrometer at the ESS. 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, as the first experiments could already confirm. The installation of the new magnets was finalized in September 2017 and since 2018 the J-NSE is back in user program. The new configuration yields an improved resolution that 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 new 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 after the refurbishment and some selected examples from the realm of soft matter dynamics that largely rely on the enhanced properties of the new J-NSE.

36

NEPOMUC – Positron Beam Facility and Instruments

Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

NEPOMUC Team

The neutron induced positron source in Munich (NEPOMUC) at FRM II/MLZ provides a positron beam with the world highest intensity of about 109 moderated positrons per second. The instruments at the positron beam facility are operated as user facility. Low-energy positron beams are applied in a large variety of experiments in condensed matter physics and materials science as well as in atomic and particle physics. The experiments performed at NEPOMUC comprise surface studies, depth dependent defect spectroscopy and fundamental research with leptonic systems. In this contribution, a review of the status of the positron beam facility with its instrumentation is given. The performance of the (remoderated) positron bam is presented and several positron beam experiments are highlighted. Recent and future developments for further improving the performance of positron beam experiments are discussed.

37

Cold Neutron Depth Profiling at the PGAA facility

Markus Trunk (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Bastian Märkisch (Department of Physics, Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Lukas Werner (Department of Physics, Technical University of Munich), Roman Gernhäuser (Department of Physics, Technical University of Munich)

Neutron Depth Profiling (NDP) is a non-destructive method to probe concentration profiles of specific light nuclides (mainly ^{6}Li, ^{10}B, ^{14}N) in different host materials. The energy loss of the charged particles produced upon neutron capture of the investigated nuclei is correlated to origin of depth and their signal intensity to concentration amount. Here, depth resolutions down to 5 nm can be achieved, depending on the sample material. The here presented N4DP setup is situated at the PGAA facility of MLZ, which provides ideal conditions for NDP: a cold white neutron flux up to 5E10 $s^{-1}cm^{-2}$, while maintaining a low background signal. Furthermore, both techniques complement each other, since NDP provides depth distributions of single nuclides within the material, whereas PGAA probes the bulk material composition.

38

The Structural and Thermal Behavior of the Thermoresponsive Polymer Poly(N-isopropylmethacrylamide) in Aqueous Solution

Chia-Hsin Ko (Department of Physics, Technical University of Munich)

Kora-Lee Claude (Department of Physics, Technical University of Munich), Dirk Schanzenbach (University of Potsdam), Bart-Jan Niebuur (Department of Physics, Technical University of Munich), Florian Jung (Department of Physics, Technical University of Munich), Jia-Jhen Kang (Department of Physics, Technical University of Munich), Henrich Frielinghaus (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Lester Barnsley (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Vitaliy Pipich (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Baohu Wu (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Alfons Schulte (University of Central Florida), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich), André Laschewsky (University of Potsdam, Applied Polymer Chemistry Group, Potsdam-Golm), Christine M. Papadakis (Department of Physics, Technical University of Munich

Compared to the well-investigated poly(N-isopropylacrylamide) (PNIPAM), Poly(N-isopropylmethacrylamide) (PNIPMAM) has a higher phase transition temperature (43 °C instead of 32 °C). This may be due to the presence of the additional methyl groups on the vinyl backbone, which lead to steric hindrance and weaken the intramolecular interactions. To understand how these effects influence the thermal and structural behavior of PNIPMAM aqueous solutions, we investigate the phase behavior of PNIPMAM in D_2O 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 °C above T_{CP}. The methyl groups in PNIPMAM lead to loosely packed large-scale inhomogeneities, and physical crosslinks already in the one-phase state. Besides, the local chain conformation of PNIPMAM is more compact than the one of PNIPAM, which is due to enhanced attractive intermolecular interactions originating from the hydrophobic moieties. In the two-phase state, PNIPMAM features larger and more hydrated mesoglobules than PNIPAM. This is due to the steric hindrance caused by the methyl groups, which weaken the intrapolymer interactions. We conclude that the methyl groups in PNIPMAM chains have a significant impact on the hydration behavior and the structural behavior around the phase transition.

39

Chemical analysis with Neutrons at the MLZ

**Zsolt Revay (Heinz Maier-Leibnitz Zentrum (MLZ),
Technical University of Munich)**
**Christian Stieghorst (Heinz Maier-Leibnitz Zentrum (MLZ),
Technical University of Munich)**
**Xiaosong Li (Heinz Maier-Leibnitz Zentrum (MLZ),
Technical University of Munich)**

Having no charge, neutrons can easily penetrate the atomic nuclei. The characteristic radiadion of the actication products is ideal for the non-destructive determination of the elemental composition.At MLZ, neutrons are used for chemical analyses in various ways. We present an overview of the different methods regarding their advantages, limitaions and applications. The focus is on the “classic” methods Prompt Gamma Activation Analysis (PGAA) and Neutron Activation Analysis (NAA). PGAA and NAA are complementary and allow for the determination of the concentrations for almost all chemical elements in many different kinds of samples. Further techniques are for instance Neutron Depth Profiling (NDP), Prompt Gamma Activation Imaging + Neutron Tomography (PGAI/NT) and Fast Neutron induced Gamma Spectrometry (FaNGaS).

40

Thiophene based Semiconductors for Organic Solar Cells

Roy Schaffrinna (Department of Physics, Technical University of Munich)

Martina Schwager (Hochschule München), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

The polymers poly(3-hexylthiophene), poly(3-thiopheneacetic acid), poly(3-thiopheneethanol) and the related copolymers are prepared starting from the respective monomer units by chemical oxidative polymerization. Graphene has also been oxidized to graphene oxide, which due to its functional groups is much more soluble in organic solvents and forms far more homogeneous layers than pure graphene and is also liquid processable. The synthesized molecules are used either as electron donor or electron acceptor in the organic solar cell and are characterized via infrared, absorption and fluorescence spectroscopy. The organic materials are electrically conductive due to their extended conjugated π-electron system and therefore require neither heavy metals / heavy metal complexes nor dopants for charge transport and can be easily deposited via spin-coating from a solution.

click here to go to
the poster list

41

Germanium-based nanostructure synthesis guided by amphiphilic diblock copolymer templating

Christian Weindl (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

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, different molar concentrations of germanium-based compounds 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 X-ray scattering (GIXS) and grazing incidence neutron scattering (GINS) are used to get further data about the formation of the inner structure in the nanoscale regime.

42

The resonant neutron spin echo spectrometer RESEDA

Christian Franz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)
Johanna K. Jochum (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Olaf Soltwedel (Physik Department, Technische Universität Darmstadt), Steffen Säubert (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Franz Haslbeck (Department of Physics, Technical University of Munich), Andreas Wendl (Department of Physics, Technical University of Munich), Leonie Spitz (Department of Physics, Technical University of Munich), Peter Böni (Department of Physics, Technical University of Munich), Christian Pfleiderer (Department of Physics, Technical University of Munich)

We report on the recent progress in the development of the longitudinal MIEZE (Modulation of IntEnsity with Zero Effort) technique at the resonant neutron spin echo spectrometer RESEDA [1] at the Heinz Maier-Leibnitz Zentrum. The key technical parameters, such as the large dynamical range and possible sample environments are discussed. Typical experimental data comprising quasi-elastic and inelastic scattering are presented to highlight the versatility of the MIEZE technique. These data include magneto-elastic coupling and crystal field excitations in $Ho_2Ti_2O_7$, the skyrmion lattice to paramagnetic transition under applied magnetic fields in MnSi, ferromagnetic criticality and spin waves in Fe as well as molecular dynamics in H_2O.

[1] C. Franz, and T. Schröder; RESEDA: Resonance spin echo spectrometer; JLSRF, 1, A1 (2015)

43

Total Reflection High-Energy Positron Diffractometer at NEPOMUC

Matthas Dodenhöft (Department of Physics, Technical University of Munich)

Artur Elovskii (Department of Physics, Technical University of Munich), Sebastian Vohburger (Department of Physics, Technical University of Munich), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Total Reflection High-Energy Positron Diffraction (TRHEPD) has been established as an ideal technique to determine the atomic positions of the topmost and immediate subsurface crystalline structure with highest accuracy. 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. However, up to now, there is just one TRHEPD setup available worldwide, which is located at the Slow Positron Facility (SPF) at the accelerator KEK in Japan.
We developed a new positron diffractometer coupled to the high-intensity positron source NEPOMUC at the research reactor FRM II. For the TRHEPD experiments, we plan to use the continuous, remoderated NEPOMUC beam, which has an intensity of ~ $5 \cdot 10^7$ e+/s. The setup features an additional transmission-type remoderator using a 100 nm thin Ni (100) foil to optionally further enhance the brightness. After the e+ beam passes a magnetic field termination, it is electrostatically focused and accelerated up to 30keV energy. We simulated the e+ trajectories to optimize the system for different beam energies and for both, remoderated and twofold remoderated beam. After the twofold remoderation, we expect a slightly converging beam with a diameter of ~1mm on the MCP. The characterization of the e+ beam and first experimental results are expected for the next reactor cycle in winter 2019.

44

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

Gaetano Mangiapia (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Martin Haese (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Nebojša Zec (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Matthias Pomm (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH, Jean-Francois Moulin (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Martin Müller (German Engineering Materials Science Centre (GEMS), Helmholtz-Zentrum Geesthacht GmbH

REFSANS is the horizontal TOF reflectometer at the MLZ in Garching. It is designed to enable reflectometry and GISANS studies of solid/liquid, solid/air and liquid/air interfaces. By using a white incident neutron beam and TOF analysis, REFSANS gives simultaneous access to a range of Q values, which is especially useful to study air-liquid interfaces or kinetic phenomena.
A six chopper system 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 possible thanks to 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 in order to tune the resolution/ intensity trade-off after the experiment.
Beside the typical sample environment, the realization of an electrochemical compact cell and the design of a humidity cell are in progress, in order to allow the investigations of electrode processes and of processes in a controlled atmosphere.

45

Lattice strain evolution of the solution heat-treated Mg-Ca alloys at room and elevated temperature under in-situ compressive deformation

Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Sihang You (MagIC, Helmholtz-Zentrum Geesthacht GmbH), Yuanding Huang (Helmholtz-Zentrum Geesthacht), Norbert Hort (MagIC, Helmholtz-Zentrum Geesthacht GmbH), Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

The addition of Ca to Mg can improve the creep resistance at elevated temperatures and the mechanical properties of Mg alloys at both room and high temperatures. In current study, the in-situ compressive deformation behaviors of solution treated Mg-0.5Zr and Mg-0.3Ca-0.5Zr alloy were investigated both at room and elevated temperatures (~200°C) at STRESS-SPEC. Cylindrical samples with 6 mm in diameter and 11 mm in length were compressed using a unique tensile/compression rig at STRESS-SPEC. Peak position and intensity variation with the compression strain were analyzed since they can indicate the evolution of lattice strain and preferred orientation, respectively. This will be related to the effect of Ca addition on the deformation modes of Mg alloys including basal slip, {10.2} twinning, prismatic slip and <c+a> pyramidal slip.

Results showed that the addition of Ca to Mg has strengthened all the deformation modes at both room and elevated temperature. However, the hardening effect of Ca on prismatic slip was much more significant than that on the other deformation modes at room temperature. All the deformation modes were softened at 200 °C, where prismatic slip and <c+a> slip got easier to be activated and basal slip carried more internal strain than that as room temperature. The alloy with Ca addition showed a better thermal stability at 200 °C due to the significantly strengthening effect of Ca solutes.

46

Structural investigation on PTX-loaded poly(2-oxazoline) molecular brushes

Jia-Jhen Kang (Department of Physics, Technical University of Munich)

Dan Gieseler (Technische Universität Dresden), Lester Barnsley (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Rainer Jordan (Technische Universität Dresden), Christine Papadakis (Department of Physics, Technical University of Munich)

Poly(2-alkyl-2-oxazoline)s (POx) feature tunable thermoresponsive properties and good biocompatibility, which make them suitable for biomedical applications, e.g. as drug carriers. In the present work, two POx-based molecular brushes, featuring PMeOx-b-PBuOx block copolymer side arms densely grafted on a poly(methacrylic acid) backbone, are investigated in aqueous solution. Whereas the hydrophobic PBuOx blocks are attached to the backbone, the hydrophilic PMeOx blocks form the periphery of the molecular brush. This architecture is suitable for drug delivery applications, since the PBuOx core can accommodate the hydrophobic anticancer drug, Paclitaxel (PTX), whereas the PMeOx shell ensures water solubility.

Using small-angle neutron scattering (SANS) at KWS-1, FRM II, the inner structure of the PTX-loaded molecular brushes with different degrees of polymerization of the backbone was investigated. The PTX/polymer weight ratio was varied from 0.1/10 to 5/10. Both brushes are elongated ellipsoids of core-shell type, with the dimension in polar direction corresponding to the backbone length. Upon PTX loading, the structure of the molecular brushes stays unchanged up to a PTX/polymer weight ratio of 1/10, whereas, above, the molecular brushes form aggregates. The brushes with higher PTX loading have significantly different structures and precipitate within few months. The stability of the drug-loaded molecular brushes is thus strongly dependent on the amount of the drug.

47

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

Martin Meven (RWTH Aachen and Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ))

Rajesh Dutta (RWTH Aachen), Andrzej Grzechnik (RWTH Aachen), Karen Friese (Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4),Forschungszentrum Jülich GmbH), Georg Roth (RWTH Aachen)

Single crystal diffraction (scd) 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.
At very high temperatures studies on $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$ brownmillerites 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]. Recent studies use a special mirror furnace developped at MLZ which allows not only temperatures > 1300 K but also atmospheres with various oxygen contents and different pressures around the sample to study their influence to the evolution of the occupation of the interstitial sites.
Last but not least a BMBF (German ministry for education and research) funded project was launched in 2016 in order to allow studys on tiny samples < 1 mm³ and to develop new pressure cells for HEiDi which can be combined with its existing low temperature equipment in order to study structural properties down to temperatures below 10 K, e.g. $MgFe_4Si_3$ compounds and their magnetic features [A. Grzechnik et al.,J. Appl. Cryst. 51, 351-356, 2018].

48

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

Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The Materials Science group consists of more than 30 people 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 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 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.

49

Highly-Regular Porous Germanium Oxide Thin Film Electrode for Lithium-ion Batteries

Suzhe Liang (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Because of high energy density, competitive working voltage, minimum self-discharge, and limited maintenance requirements, rechargeable lithium-ion batteries (LIBs) have been applied in various fields and regarded as the most promising power devices in the future. Due to high theoretical capacity (2152 mAh g^{-1}), germanium oxide (GeO_2) is regarded as a promising alternative anode material for LIBs. However, GeO_2 suffer from volume expansion during charge and discharge, leading to a rapid capacity fading. Creating hollow or porous structure is an effective strategy to improve the cycling stability of germanium oxide anode because it can provide enough void space to accommodate volume changes of germanium oxide. Herein, we propose a novel method to synthesize highly-regular porous GeO_2 tin film anode materials assisted with the block copolymer. Polymer/inorganic nanocomposites can be obtained via a microphase separation process in a mixture solution of mixing block copolymer and precursor of metal oxide. The morphology of as-prepared porous germanium oxide tin film anodes could be characterized by scanning electron microscopy (SEM) partially and grazing incidence small-angle X-ray scattering (GISAXS) integrally. Furthermore, in-operando SAXS or Small-angle neutron scattering (SANS) measurements can be applied to investigated the evolving nanoscale morphology of electrode during charge and discharge processes.

50

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

Xiaohu Li (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Soria Sergio (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Weimin Gan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

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

51

What is the initial stage of degradation mechanism for perovskite solar cells?

Renjun Guo (Department of Physics, Technical University of Munich)

Wei Chen (Department of Physics, Technical University of Munich), Lennart Reb (Department of Physics, Technical University of Munich), Shanshan Yin (Department of Physics, Technical University of Munich), Kerstin Wienhold (Department of Physics, Technical University of Munich), Manuel Scheel (Department of Physics, Technical University of Munich), Benjamin Predeschly (Department of Physics, Technical University of Munich)

Mixed organic-inorganic hybrid perovskite solar cells have shown a promising future because of their outstanding photoelectric performance. The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached the champion value of 24.2 %, making this technique competitive with commercial silicon solar cells. Despite all these 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.
In addition, the rapid developing progress in the fabrication of PSCs has not accompanied the development of start-of-the-art characterization methods. Current degradation research on PSCs is performed by simple current-voltage measurement. Therefore, it is necessary to introduce new characterization tools for analyzing the degradation mechanisms of PSCs. We investigated initial-stage degradation processes of different device architectures of PSCs under illumination condition with in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small-angle X-ray scattering (GISAXS). With this approach, we are able to follow the evolution of characteristic structures and of the inner morphology under illumination. After understanding the degradation mechanisms for different device architectures, potential solutions could be found to suppress degradation.

52

QENS and in-situ SANS Investigations of Complex Hydrides

Neslihan Aslan (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH)

Wiebke Lohstroh (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Claudio Pistidda (German Engineering Materials Science Centre (GEMS), Helmholtz-Zentrum Geesthacht GmbH), Klaus Pranzas (German Engineering Materials Science Centre (GEMS), Helmholtz-Zentrum Geesthacht GmbH), Martin Müller (German Engineering Materials Science Centre (GEMS), Helmholtz-Zentrum Geesthacht GmbH)

With hydrogen as energy carrier, hydrides are in the focus of research for the application of energy storage and energy transportation. Within the complex hydrides, the metal hydride composite $Mg(NH_2)_2$ + LiH has recently gained in importance because of good properties for reversible hydrogen storage. $Mg(NH_2)_2$ + LiH has faster de- and rehydrogenation kintetics with the addition of $LiBH_4$. So far $Mg(NH_2)_2$ + LiH + $LiBH_4$ is a good candidate to be used for hydrogen storage with the high capacity (ca. 4 wt%) and good reversibility.
To understand the effect of the LiBH4 additive on the kinetics, neutron scattering experiments were applied at the Heinz Maier-Leibnitz Zentrum (MLZ). With this poster we present the investigated quasielastic neutron scattering (QENS) and in-situ small angle neutron scattering (SANS) measurements.
At the TOFTOF instrument the Time-of-Flight spectroscopy of $Li_4BH_4(NH_2)3$ was investigated, which is an intermediate of the dehydrogenated $Mg(NH_2)_2$ + LiH + $LiBH_4$-system. This product showed in the QENS measurement high degree of freedom for rotational and transversal motions. With the high mobility of the BH_4-tetrahedron, the fast absorption/desorption kinetics of the complex hydrides are explained.
In-situ SANS of $Mg(NH_2)_2$ + LiH + $LiBH_4$ at SANS-1 instrument was measured. The analyzed sizes of the nanoparticles are preserved after hydrogenation/dehydrogenation reactions. In addition, a model for these reactions are proposed based on the in-situ measurements.

53

Self-assembly of large magnetic nanoparticles in ultrahigh molecular weight linear diblock copolymer films

Wei Cao (Department of Physics, Technical University of Munich)

Senlin Xia (Department of Physics, Technical University of Munich), Xinyu Jiang (Department of Physics, Technical University of Munich), Michael Appold, Matthias Opel (Department of Physics, Technical University of Munich), Markus Gallei (Universität des Saarlands), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron DESY), Stephan V. Roth (Deutsches Elektronen-Synchrotron DESY), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

The preparation of block copolymer nanocomposite films that consist of nanoparticles (NPs) with diameters (D) of more than 10 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) diblock copolymer was spin-coated as a template for the self-assembly of large iron oxide NPs (D = 27 nm), and the morphology of hybrid nanocomposites was governed by the concentration (c) of the iron oxide NPs. Via hydrogen bonding between the carboxylic acid groups on iron oxide and the PMMA side chains of the diblock copolymers, the NPs were selectively incorporated inside the PMMA spheres. Due to the rearrangement of the PMMA chains for accommodating the NPs, well-ordered spherical nanostructure were readily generated at low NP concentrations (c = 0.5 wt%). Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading. All hybrid films show ferromagnetism at room temperature.

54

In-situ printing of PBDB-T-SF:IT-4F for application in high-efficiency organic solar cells

Kerstin Wienhold (Department of Physics, Technical University of Munich)

Volker Körstgens (Department of Physics, Technical University of Munich), Sebastian Grott (Department of Physics, Technical University of Munich), Xinyu Jiang (Department of Physics, Technical University of Munich), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron DESY), Stephan Roth (Deutsches Elektronen-Synchrotron DESY / KTH), Peter Mueller-Buschbaum (TDepartment of Physics, Technical University of Munich)

Printing of active layers of organic solar cells is one possible way to overcome the challenge of up-scaling, which is the main drawback in the field of organic photovoltaics on their way to marketability. Thin layers of PBDB-T-SF:IT-4F, a conjugated high-efficiency polymer and a non-fullerene small molecule acceptor, 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 and drying kinetic of active layers.

55

Cononsolvency in PNIPAM-based block copolymer thin films

Christina Geiger (Department of Physics, Technical University of Munich)

Tobias Widmann (Department of Physics, Technical University of Munich), Lucas Kreuzer (Department of Physics, Technical University of Munich), Gaetano Mangiapia (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Cristiane Henschel (University of Potsdam), André Laschewsky (University of Potsdam), Christine M. Papadakis (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

The diblock copolymer PMMA-b-PNIPAM forms micelles in aqueous solution that exhibit a reversible shell collapse transition at the lower critical solution temperature (LCST). This thermo-response can be moderated by introducing organic cosolvents such as methanol, ethanol or acetone. In thin film configuration, their multi-responsive behavior makes NIPAM-based polymers promising systems for vapor-sensitive nanosensors and actuators. We prepare thin films with a large PNIPAM block and perform swelling experiments in a custom chamber. The film response is probed for mixed vapors of different solvent and cosolvent content, while the temperature is held constant in order to purely probe the cononsolvency effect. Morphological changes, as well as the swelling kinetics related to the uptake of solvent and cosolvent into the film, concentration gradients and the development of swelling ratio and refractive index are investigated with a focus on spectroscopic reflectance (SR) and in-situ time-of-flight neutron reflectometry (TOF-NR). Running sequential experiments with protonated and deuterated compounds allows us to extract the individual distributions of solvent and cosolvent in the film by contrasting SLD profiles from static TOF-NR curves. SR can be used to monitor the film thickness in real time as well as to use as a feed parameter in batch fits of kinetic TOF-NR data. First results show that cononsolvency-related behavior is transferrable from solution to thin film systems.

56

Small-Angle Neutron Scattering Instrument SANS-1 at MLZ

Sebastian Muehlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

André Heinemann (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH), Apostolos Vagias (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

We present the features of the instrument SANS-1 at MLZ, a joint project of Technische Universität München and Helmholtz Zentrum Geesthacht. Measurements of the beam profile, divergence, flux and polarization are given for various positions along the instrument and agree well with simulations. SANS-1 features two interchangeable velocity selectors with 10% and 6% $\Delta\lambda/\lambda$ and a TISANE 14-window double-disc chopper. This combination allows tuning flux, resolution, duty cycle and frame overlap, including time resolved measurements with repetition rates up to 10 kHz. A key feature is the large accessible Q-range facilitated by the sideways movement of the detector. Particular attention is paid to effects like tube shadowing, finite tube wall thickness and anisotropic solid angle corrections, that arise due to large scattering angles on an array of single ^{3}He tubes, where a standard cos3 solid angle correction is no longer valid.

Dedicated to hard matter, materials science and magnetism, SANS-1 features a flexible, spacious sample area with a heavy duty goniometer and unique sample environment like a set of magnets, ovens and a bespoke dilatometer. We show some extreme examples and prospects for future experiments, e.g. to investigate the onset of crystallization in magnetic materials and a future high field magnet project. Finally we present the polarization analysis option that combines a new compensated MEOP and an integrated RF-flipper together with a 2.2 T magnet.

57

Neutron & X-ray diffraction studies of graphite anodes conducted at MLZ

Stefan Seidlmayer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Jörn Wilhelm (Department of Electrical and Computer Engineering, Technical University of Munich), Simon Erhard (Department of Electrical and Computer Engineering, Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Andreas Jossen (Department of Electrical and Computer Engineering, Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Current state of the art lithium ion batteries typically use graphite as an anode material. Understanding the dynamical processes during lithiation and delithiation is crucial for comprehending performance and degradation. Especially due to the detrimental effects of fast charging or charging at low temperatures. Many aging processes, like lithium plating, depend intrinsically on the lithiation properties. Lithium plating enhances cell aging and imposes a security issue in commercial cells [1]. Detailed understanding of the material properties and the dynamic lithiation processes in commercial type cells is necessary to avoid security issues and performance deterioration due to occurrence of Li plating or phase inhomogeneity. In our studies of graphite/NMC cells with operando neutron diffraction we found that intermittent Li plating and phase inhomogeneity in graphite anodes can be observed even under unexpectedly mild conditions, although the effects are often hidden due to the fast relaxation processes at room temperature [1]. Within the ExZellTUM II project (funded by BMBF, grant no. 03XP0081), we recently studied the temperature and current density dependence and the lithiation dynamics with neutron diffraction [2]. By combining neutrons with post-mortem x-ray diffraction [3] the lithiation process in large batteries can be better understood.

[1] Zinth et al., JPS, (2014), 271, 152.

[2] Wilhelm, et al., JES, (2018), 165, A1846.

[3] Wilhelm, et al., JPS, (2017), 365, 327.

58

Influence of solvent on the morphology and optical properties of printed active layers based on PBDB-T-SF:IT-4F for application in organic solar cells

Daniel Steger (Department of Physics, Technical University of Munich)

Kerstin Wienhold (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Polymer-based organic solar cells (OSCs) are of rising interest in research and industry due to their potential advantages such as light-weight, flexibility, semi-transparency and low production cost. The power conversion efficiency of OSCs has been significantly improved in recent years, by now up to about 15 %. Yet scalability is a still major factor to make OSCs economically viable. Producing the active layer via thin-film printing is a promising approach as it facilitates the fabrication of large-area organic solar cells compared to the more commonly used spin-coating technique. Still this technology has to be further investigated and printing parameters have to be optimized to increase the resulting quality. The active layer of OSCs consists of a blend of a polymer donor material and a non-fullerene acceptor material. In this work, the polymer PBDB-T-SF and the non-fullerene small molecule acceptor IT-4F with reported efficiencies up to 13 % have been investigated. As the PCE of OSCs greatly depends on the morphology of the active layer, factors influencing the morphology, such as the used solvent, are of great interest. Effects of different solvents can be studied by looking at the absorption characteristics via UV/VIS spectroscopy in solution as well as in a thin film. The morphology itself can be investigated via surface probing techniques such as AFM or grazing incidence small angle x-ray scattering (GISAXS) to gain statistical information about the inner structure.

59

Bio-hybrid thin films for templating titania nanostructures

Julian Heger (Department of Physics, Technical University of Munich)

Anna-Lena Öchsle (Department of Physics, Technical University of Munich), Nian Li (Department of Physics, Technical University of Munich), Shanshan Yin (Department of Physics, Technical University of Munich), Calvin Brett (KTH, Royal Institute of Technology), Wiebke Ohm (Deutsches Elektronen-Synchrotron (DESY)), Stephan Roth (Deutsches Elektronen-Synchrotron (DESY)), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Polymer based films are of high practical use, e.g. as coatings, biomedical applications or flexible electronics. In combination with inorganic materials, this films form interesting hybrid systems of elevated performance, joining advantages of both material classes: Solution processing providing possibilities of cheap industrial fabrication and inorganic characteristics like enhanced electrical, magnetic or drug properties. A novel and promising approach in the field of polymeric soft matter is to substitute these synthetic polymers with environmental biopolymers, such as proteins. Being water soluble, earth abundant and non-toxic, they open a way to green soft matter processing. We are interested in the structure directing properties of the bovine whey protein ß-lactoglobulin (ß-lg) for thin titania films. For this, denatured ß-lg is mixed with established titania precursors to form a sol-gel, which can be eventually deposited. Spray deposition is chosen as a technique of low material wastage. Calcination of the as deposited films combust the biopolymer template and introduces crystallinity into the nanostructured titania. By backfilling the remaining scaffold with the organic semiconductor P3HT, photon sensors can be created. Grazing incidence small-angle X-ray scattering (GISAXS) reveal the film formation in situ during spray coating, as well as in operando morphological degradation of the sensor. GISAXS is complemented by real space imaging, e.g. electron microscopy.

60

EMIM-DCA post-treatment of semi-conducting PEDOT:PSS polymer thin films to improve their thermoelectric properties

Anna-Lena Öchsle (Department of Physics, Technical University of Munich)

Julian Heger (Department of Physics, Technical University of Munich), Nian Li (Department of Physics, Technical University of Munich), Shanshan Yin (Department of Physics, Technical University of Munich), Hartmut Stadler (Bruker), Sigrid Bernstorff (Elettra Sincrotrone Trieste S. C. p. A.), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

In times of constantly increasing energy demand, climate change and scarcity of fossil resources the need for renewable energies and the reduction of energy dissipation is of immense importance. Therefore, thermoelectric materials are of great interest in terms of waste heat recovery and the use of solar thermal energy, as they enable the direct conversion of a temperature gradient into electrical power. In particular, thermoelectric polymers are attractive, because in contrast to inorganic materials they are low or non-toxic, lightweight, flexible and enable a low-cost solution based processability. An often used way to evaluate thermoelectric properties is the so-called power factor $PF=S^2\sigma$. This parameter depends on the Seebeck coefficient S and the electrical conductivity σ, which are affected by the electronic and morphological features of the polymer. We are investigating methods to improve S and σ. Post-treatment of fabricated PEDOT:PSS thin films with ionic liquids like EMIM-DCA influences the electronic as well as the morphological polymer properties. Thus, we are able to increase S and σ simultaneously, leading to an improvement of the power factor. With measurements of parameters such as S, σ, absorbance, layer thickness and determination of the structure, the underlying morphology-function relationship is determined.

61

Revealing the formation of sputter deposited metal nanolayers on functional polymer thin films for lithium-ion batteries

Simon J. Schaper (Department of Physics, Technical University of Munich)

Franziska C. Löhrer (Department of Physics, Technical University of Munich),Volker Körstgens (Department of Physics, Technical University of Munich), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron (DESY)), Pallavi Pandit (Deutsches Elektronen-Synchrotron (DESY)), Alexander Hinz (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), Oleksandr Polonskyi (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft),Thomas Strunskus (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), Franz Faupel (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), Stephan V. Roth (Deutsches Elektronen-Synchrotron (DESY) / KTH), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible, and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-film morphologies on the nanoscale and offers a superior adhesion of the deposited material. The successful use to reveal the growth of gold on polymer thin films, motivates the use of in situ grazing-incidence small-angle X-ray scattering (GISAXS) to investigate the formation, growth, and self-assembled structuring on polymer thin films for LIBs. Post deposition ellipsometry measurements provide additional information about intermixing layers and their composition. Different polyethylene oxide based polymer films are compared with respect to the metal layer growth.

62

KWS-1: High-flux SANS instrument with polarization analysis

Artem Feoktystov (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Lester Barnsley (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Marie-Sousai Appavou (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Zahir Salhi (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Earl Babcock (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Henrich Frielinghaus (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

The KWS-1 small-angle neutron scattering instrument is operated by JCNS at MLZ. 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 and a high resolution owing to its neutron selector with an optional double-disc chopper to reduce the wavelength spread down to $\Delta\lambda/\lambda$ = 1% [1]. This allows study of feature sizes from 10 to 9000 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. This is a highly flexible instrument with many possibilities and options available for users.

A suite of sample environments is available to allow users to study magnetic systems down to cryogenic temperatures and in horizontal or vertical fields up to 5 T. A custom-designed, non-magnetic hexapod at the sample position can carry up to 550 kg of useful load, and can allow flexible positioning and orientation of heavy sample environments for measurements either in transmission or grazing-incidence small-angle neutron scattering (GISANS) geometries. Polarization analysis option can be used to clearly separate the magnetic and nuclear scattering contributions. Recent upgrades to the instrument, in particular, a new option for in-situ polarization of a ^{3}He neutron spin filter, allowing for time-independent analyzing efficiency of post-scattered neutrons will be presented.

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

click here to go to the poster list

63

Printed organic thin films for photovoltaic applications – a morphology study

Sebastian Grott (Department of Physics, Technical University of Munich)

Rodrigo Delgado Andrés (Department of Physics, Technical University of Munich), Volker Körstgens (Department of Physics, Technical University of Munich), Kerstin Wienhold (Department of Physics, Technical University of Munich), Xinyu Jiang (Department of Physics, Technical University of Munich), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron (DESY)), Stephan Roth (Deutsches Elektronen-Synchrotron (DESY) / KTH) Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

The conversion of energy out of sunlight is an indisputably promising possibility to tackle the problem of the continuously growing energy demand. Thereby, organic photovoltaics (OPVs) have attracted considerable attention, due to their outstanding characteristics, such as potential low-cost fabrication, high throughput, light weight, flexibility and easy processability. Fabrication techniques for OPVs devices vary depending on the used materials and include spray casting, inkjet printing and roll-to-roll printing. Among these, the scalability of the printing processes makes them attractive for industrial application, since it is possible to deposit the donor:acceptor blend of the active layer out of one solution. In this study, the influence of different ratios of donor and acceptor are explored for thin film bulk heterojunction OPVs deposited by printing methods. In order to characterize these solar cells their current-voltage characteristics as well as their absorbance spectra are measured. Additionally, the inner morphology of the active layers is probed with advanced scattering techniques, such as grazing incidence small angel X-ray scattering (GISAXS) and grazing incidence wide angel X-ray scattering (GIWAXS), to correlate structural information with the obtained photoelectrical properties of the devices. This correlation is needed to further optimize the processing parameters to enhance power conversion efficiencies and the overall performance of organic solar cells.

64

Critical scattering in classical and quantum critical systems

Heiko Trepka (Max Planck Institute for Solid State Research)

Thomas Keller (Max Planck Institute for Solid State Research), Matthias Hepting (Max Planck Institute for Solid State Research), Kuo Feng Tseng (Max Planck Institute for Solid State Research), Oliver Stockert (Max Planck Institute for Physics of Solids), Bernhard Keimer (Max Planck Institute for Solid State Research)

We report on a study of critical scattering in classical and nearly quantum critical antiferromagnets (AFMs). The energy width of the critical scattering was determined by high-resolution neutron spin-echo at TRISP at the MLZ in Munich. The classical systems studied include the s=5/2 AFMs Rb_2MnF_4 and MnF_2 with quasi 2D and 3D spin interactions, respectively. Both compounds are Heisenberg AFMs with a small uniaxial anisotropy resulting from dipolar spin-spin couplings, which leads to a crossover in the critical dynamics close to the Neel-Temperature (TN). By means of our high-resolution measurement we were able to identify the dynamical critical exponents z for both longitudinal and transverse fluctuations. Thus discrepancies between experiment and theory observed in previous three-axis studies could be resolved. For a study of quantum critical systems, we chose the $CeCu_{(6-x)}Au_{(x)}$ series, which exhibits a quantum critical point at x=0.1 seperating nonmagnetic (x<0.1) and magnetically ordered ground states (x>0.1). First measurements at $CeCu_{5.8}Au_{0.2}$ (TN=0.22K) show a hitherto unexplained dynamical critical exponent.

65

Synthesis of Mesoporous TiO_2 by using PS-b-P4VP as template block co-polymer: Fabrication and Analysis

Magdalini Spyranti (Department of Physics, Technical University of Munich)

Nian Li (Department of Physics, Technical University of Munich), Simon Schaper (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Mesoporous titania have been extensively studied owing to their high surface area, unique electronic and optical properties and applications in photocatalysis and dye sensitized solar cells[1]. An optimal mesopore size of the nanostructured titania film plays a significant role in the device efficiency improvement.

In this work, the bottom up approach of sol-gel synthesis has been used to fabricate titanium oxide films. As a template the diblock copolymer polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) is used to define the structure and titanium tetra isopropoxide (TTIP) as the precursor. The amphiphilic block copolymer PS-b-P4VP undergoes phase separation and self-assembly due to a good-bad solvent pair, namely N,N-dimethylformamide (DMF) and acetic acid (CH_3COOH). By adjusting the weight ratio of acetic acid and TTIP, the mesoporous sponge-like titania films are obtained after template removal by calcination.

The surface and inner morphology are explored by optimal microscopy (OM), scanning electron microscopy (SEM) and grazing incidence small-angle X-ray scattering (GISAXS). Furthermore, the anatase phase of the crystalline titania films is verified by X-ray diffraction. The transmittance is investigated by ultra-visible spectroscopy (UV-vis).

[1] Yonghui Deng, Jing Wei, Zhenkun Sun and Dongyuan Zhao, Chem. Soc. Rev., 2013, 42, 4054

66

Wearable Electronic Skin based on Triboelectric and Luminescent Effect for Pressure and Tensile Sensing

Tianxiao Xiao (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Electronic skin (E-skin) as the medium between ambient environment and bionic robots is an advanced technology that provides an electronic readout or even produces a visualized response that can be easily captured for post-processing. Since this concept birth, different electronic skins have been fabricated and utilized for various sensing applications, such as pressure, humidity, temperature et al. However, to mimic human skin better, combining more sensing capabilities into one E-skin system is highly in demand.

In this work, we fabricated a new type of wearable E-skin system based on triboelectric and luminescent effect for both pressure and tensile sensing. This device consists of a PDMS-based single-electrode mode triboelectric nanogenerator as a pressure sensor and a luminescent layer for tensile sensing. Here, the luminescent effect is realized by adding CdSe/CdS quantum rods (QRs) into PDMS film, which can be excited under visible light. The sensitivity of the pressure sensor is enhanced by surface morphology. GISAXS/SAXS are used to characterize both the distribution of QRs and the surface morphology of PDMS film.

67

Studies on VDM alloy 780 Premium with standard heat treatments using synchrotron radiation

Lu Qin (Department of Physics, Technical University of Munich)

Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Andreas Stark (Institute of Materials Research, Helmholtz-Zentrum Geesthacht), Bodo Gehrmann (VDM Metals International GmbH, Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Alloy 718 has been widely used in gas turbine and related applications due to its good mechanical properties and structural stability at elevated temperatures (650 °C). The operation temperature of the alloy 718 is limited because of the transformation of the metastable strengthening γ'' phase to stable δ phase at high temperature. A new 718-type Ni-Co based superalloy VDM 780 Premium was developed for higher temperature application. In comparison to alloy 718, the main composition change in VDM 780 is essential replacement of Fe by about 25% Co and a higher Al content in combination with a lower Ti content.
Synchrotron measurements were performed on bulk samples of VDM 780 Premium with standard heat treatment, i.e. the solution heat treated at 980 °C/1.5 h + 720 °C/8 h/FC + 620 °C/8 h/AC. The diffraction patterns were taken (a) during heating and cooling down after 0.5 at the highest T (1040 °C) and (b) during heating and at different holding temperatures (at 970,980 and 990 and 1020,1030 and 1040 °C). The Rietveld refinement of the measured diffraction patterns allowed (1) the identification of all phases present in the sample, γ matrix, γ' hardening phase, NbC and δ and η high temperature phases; (2) the evolution of the cell parameters and misfit with temperature, and (3) solvus and precipitation temperatures determination.

68

Development of a new testing device for in-situ microstructural characterization under mechanical and thermal loading

Frank Kümmel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Johannes Munke (Department of Physics, Technical University of Munich), Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The goal of this project (BMBF INA780) is the implementation of an innovative testing machine to perform deformation experiments at high temperatures at various instruments at the research neutron source Heinz Maier-Leibnitz. With neutron diffraction, small angle scattering and radiography (tomography) it is possible to investigate forming phases, their volume fractions as well as size and shape, dislocation density, textures, recrystallization processes and crack propagation. The field of possible loading cases of the newly developed testing machine is manifold. In the current state, uniaxial tensile and compression experiments can be performed. But also more complex loading cases like crack propagation tests in CT-samples or cyclic loading can be implemented. The testing temperature can be varied from room temperature up to 1200 °C. In addition, a controlled cooling of the samples by pressured gas will also be possible. Due to a completely closed casing, the tests can be conducted in vacuum or special atmospheres.
This testing machine offers a unique possibility for the development of newly high-performance materials. One the one hand, it is possible to measure the microstructural parameter of materials within the thermo-mechanical process chain from forming to the subsequent heat treatment steps. On the other hand, the material behavior under service conditions can also be investigated to predict the failure criterion and the service life of components.

click here to go to
the poster list

69

KWS-2 - small angle neutron diffractometer

Aurel Radulescu (Jülich Centre for Neutron Science (JCNS) at
Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Christian Lang (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Marie-Sousai Appavou (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

KWS-2 is a classical small angle neutron 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 1 x 10^{-4} and 0.5 $Å^{-1}$.
The instrument is designed for high intensity studies with a broad q-range, covering meso-scopic structures and their changes due to kinetic processes in the fields of soft condensed matter, chemistry, and biology.
The high neutron flux, comparable with leading SANS instruments worldwide, and the possi-bility to measure samples with large diameter (up to 5 cm), employing the MGF2 lenses, allow for high intensity and time-resolved studies.
In special cases, the resolution can be improved by using a double-disc chopper with adjust-able openings. This allows for a relative change of the wavelength spread between 2 and 20 %. In this way, the instrument can be flexibly adjusted to the needs of different experiments. Structural details can be characterized better and the beam characteristic can be adjusted. Furthermore, the effects of chromatic aberration of the lenses and gravitation effects can be minimized.
A broad range of side-instruments including rheometer, stopped-flow, high-pressure cells, and a newly developed size exclusion chromatography device with in-situ UV-Vis spectroscopy, specially designed for studying aggregation prone proteins, allow for highly individualized studies of soft matter samples.

70

3D printed humidity chamber for neutron scattering experiments

Tobias Widmann (Department of Physics, Technical University of Munich)

Lucas Kreuzer (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

The investigation of stimuli-responsive organic thin films, which are sensitive to changes in temperature, humidity or other conditions, requires defined environmental conditions at the sample position. Especially in combination with neutron scattering techniques, such as grazing incidence small angle neutron scattering (GISANS) or neutron reflectometry (NR), high re-quirements to the sample environment are existing. In the framework of the FlexiProb project, which plans a flexible and interchangeable sample environment system for various neutron experiments at the European spallation source (ESS), we designed a sample environment for neutron scattering experiments on thin films in varying environmental conditions. Its core is a 3D printed aluminum chamber connected to an external gas- and fluid-flow. The chamber is designed spherical to reduce internal condensation and to provide a uniform heat distribution around the sample. For that purpose, fluidic channels through the chamber walls and lid help to minimize heat gradients throughout the chamber. The gas-flow can be composed of up to three different gas streams, where each one can be controlled individually. This provides pure gas or solvent atmospheres, or enables mixtures of different gas composition to the desired specifica-tions. The developed setup is planned to be used at other neutron instruments as well and was already successfully tested at the REFSANS instrument at the MLZ.

click here to go to the poster list

71

Formation of a micrometer positron beam at the Scanning Positron Microscope

Johannes Mitteneder (Universität der Bundeswehr München)

Marcel Dickmann (Universität der Bundeswehr München), Werner Egger (Universität der Bundeswehr München), Ricardo Helm (Universität der Bundeswehr München), Günther Dollinger (Universität der Bundeswehr München), Gotfried Kögel (Universität der Bundeswehr München)

To investigate inhomogeneous defect distributions e.g. close to fatigue cracks or dispersive alloy with positron annihilation lifetime spectroscopy a pulsed positron beam with a diameter in the range of 1 µm and with a time resolution in the order of 250 ps is needed.
To this aim the Scanning Positron Microscope (SPM) was built at the Universität der Bundeswehr. To overcome the limit of low count-rates and corresponding exceedingly long measurement times the SPM is transferred to the intense positron source NEPOMUC at the MLZ in Garching. To connect the SPM to NEPOMUC a special interface has been constructed. It consists of a series of pulsing elements, a remoderation stage and a new positron elevator to change the potential energy of the pulsed positron beam.
The radio frequency positron elevator has been tested, which is the final step of the SPM interface. The elevator compensates the loss of potential energy, lost by the implantation of the positron remoderation processes. Since the elevation does not influence other beam parameters, the brightness and the time structure of the positron beam is conserved. This device allows also keeping both, the source and the sample, at the same electrical potential.

72

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

Dmitry Gorkov (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Georg Waldherr (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Alexander Grünwald (Institut Laue-Langevin (ILL)), Jonas Stein, Stefan Giemsa (Department of Physics, Technical University of Munich), Peter Böni (Department of Physics, Technical University of Munich), Markus Braden (Universität zu Köln)

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.

click here to go to
the poster list

73

Bambus: a new inelastic neutron multiplexed analyzer for Panda at MLZ

Alexandre Bertin (Institut für Festkörperphysik, Technical University Dresden)

Joshua Lim (Institut für Festkörperphysik, Technical University Dresden), Petr Cermak (Department of Condensed Matter Physics, Charles University), Igor Radelytskyi (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Astrid Schneidewind (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Dmytro Inosov (Institut für Festkörperphysik, Technical University Dresden)

Cold triple-axis spectrometers (TAS) are dedicated to the investigation of low-energy excitations in a wide area of condensed matter physics, from quantum magnetism to unconventional superconductors. This technique allows us to measure individual points in the large (Q,E) space for one instrument setting, at low temperatures and high magnetic fields. New engineering solutions are being developed in order to increase the useful signal on TAS. With this purpose, the multianalyser Bambus is being constructed at the cold TAS Panda at MLZ, led by TU Dresden and in cooperation with JCNS. Its concept lies in collecting data at a certain energy transfers along a curved path in Q space, with the aim to construct broad reciprocal space maps at multiple energy transfers in a reliable, easy-to-use setup without movable axes. Hence, experiments will provide an overview in a large (Q,E) space, in order to get insights of broad features at low energy or study complex dispersion laws. Because this spectrometer is designed as a complementary module, a fast switch between the two setups is foreseen. This project received a new financial support from the BMBF project 05K19OD1 for the period 2019-2021, aiming for the commissioning of the instrument and software development. For the latter purpose, a collaboration has been initiated among European TAS multiplexing teams in order to implement a common, user-friendly tool for instrumental resolution calculation, data visualization and analysis.

74

Morphology Tuning of ZnO Nanostructures for Hybrid Solar Cells

Ting Tian (Department of Physics, Technical University of Munich)

Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Hybrid solar cells have attracted great attention due to the advantages of their short payback time, high stability and flexibility, which results from the combination of inorganic and organic materials. For hybrid solar cells, DSSCs (solid-state dye-sensitized solar cells) and HBSCs (hybrid bulk-heterojunction solar cells) are mostly explored. For both of these kinds of solar cells, nanostructured ZnO is used as an electron transport material to provide a large interface area for exciton separation and electron extraction to their corresponding electrode. Therefore, the morphology of the ZnO films plays a critical role in improving the photovoltaic performance of ZnO based solar cells. Here, mesoporous ZnO nanostructures are synthesized via a diblock copolymer assisted sol-gel approach. For tuning the morphology of the ZnO films, characteristic parameters, such as the composite ratio of the materials, the deposition method, and the annealing temperature are investigated during synthesis. Subsequently, the surface morphology and the inner morphology are probed using scanning electron microscopy (SEM), atomic force microscopy (AFM) and grazing-incidence small-angle X-ray scattering (GISAXS), respectively. Based on controlled nanostructured ZnO films, all ssDSSCs or HBSCs are prepared and photovoltaic performance is investigated.

75

Influence of printing temperature on the efficiency of organic solar cells

Linus Huber (Department of Physics, Technical University of Munich)

Kerstin Wienhold (Department of Physics, Technical University of Munich), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Today, one of the biggest challenges is the development of carbon-neutral energy technologies. Solar cells have been a frontrunner for eco-friendly energy conversion for a long time, but in search for better energy conversion and cheaper production, new materials and production techniques need to be put forward. Printable-thin-film solar cells could lower production-cost by means of a high scale-up potential and an easier production process. They can also yield high efficiencies, are of lighter weight, flexible and semitransparent. This suggests a wide variety of possible applications, where silicon-solar cells seem to be less applicable. Controlling the temperature of the printing process could lead to better efficiencies and a deeper understanding of the polymer-structures dependence on temperature. Four different printing temperatures are studied and evaluated using UV-Vis, photoluminescence and AFM.

76

The high resolution neutron backscattering spectrometer SPHERES

Michaela Zamponi (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

Daria Noferini (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Marina Appel (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)

The SPectrometer for High Energy RESolution (SPHERES) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It provides high energy resolution with a good signal-to-noise ratio. Over the recent years different components of the instrument have been upgraded to further improve the instrument performance.
SPHERES enables investigations on a broad range of scientific topics. 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. Hence it is well suited to investigate dynamics in various soft matter systems like polymers or proteins. Other typical applications include molecular reorientations and rotational tunneling, diffusion processes in various systems or relaxation in viscous liquids.

77

Simultaneous injection of positrons and electrons – progress towards a pair-plasma at NEPOMUC

Markus Singer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Eve. Stenson (Max-Planck-Institute for Plasma Physics, Technical University of Munich and University of California), Juliane Horn-Stanja (Max Planck Institute for Plasma Physics), Stefan Nissl (Max Planck Institute for Plasma Physics), Thomas Sunn-Pedersen (Max Planck Institute for Plasma Physics), Haruhiko Saitoh (University of Tokyo), Marcel Dickmann (Universität der Bundeswehr München), Matthew Stoneking (Max Planck Institute for Plasma Physics), James R. Danielson (University of California), Clifford M. Surko (University of California)

A pair-plasma, a system where both the positively and negatively charged particles have the same mass, is predicted to possess unique physical properties. The APEX collaboration attempts to magnetically confine the first low-temperature electron-positron pair plasma in the magnetic field of a levitated superconducting coil. In a prototype experiment, positrons provided by the NEPOMUC facility are magnetically guided towards our confining field created by a supported permanent magnet. Perpendicular electric and magnetic fields at the injection

click here to go to
the poster list

port provide a drift to inject the positrons across magnetic field lines. Extensive investigations of the large parameter space spanned by electric and magnetic field configurations deepened the understanding of the injection process and resulted in injection efficiencies of 100% [1] and confinement times exceeding one secondb[2]. To create the first mixture of positrons and electrons in our device, a compact electron source placed upstream forms a second beam propagating parallel to the positron beam. A successful co-injection and detection of both particles was demonstrated, while using conditions optimized for positron injection. This represents an important step towards the goal of a confined pair-plasma. An overview of this project as well as future prospects will be presented in this contribution.

[1] E. V. Stenson, et.al., Phys. Rev. Lett. 121, 235005 (2018).

[2] J. Horn-Stanja, et al., Phys. Rev. Lett. 121, 235003 (2018).

78

ErwiN in the making - a Fast Neutron Powder Diffraction Option

Michael Heere (Karlsruher Institute of Technology (KIT))

The need for rapid data collection and studies of small sample volumes in the range of mm^3 are the main driving force for the concept of a high-throughput monochromatic diffraction instrument at the Heinz Maier-Leibnitz Zentrum (MLZ). A large section of reciprocal space will be addressed with sufficient dynamic range and µs time-resolution while allowing for a variety of complementary sample environments. The medium-resolution neutron powder diffraction (NPD) option for “Energy research with Neutrons” (ErwiN) at the research reactor Munich is foreseen to meet future demand. ErwiN will especially be suited for addressing structural studies and its uniformity of energy-related systems and materials by using simultaneous bulk/spatially resolved NPD. A set of useful experimental options will be implemented enabling time-resolved studies, rapid parametric measurements as a function of external parameters or studies of small samples using an adapted radial collimator. The proposed powder diffraction option ErwiN will bridge the gap in functionality between the high-resolution powder diffractometer SPODI and the time-of-flight diffractometers POWTEX and SAPHIR.

79

A New Measuring Cell for Operando Neutron Diffraction on Li-Ion Battery Cathode Materials

Daniel Sørensen (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Michael Heere (Karlsruher Institute of Technology (KIT)), Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The use of operando diffraction has taken a major step forward, in no small part due to the increase in flux at large scale facilities such as synchrotrons and neutron spallation sources. While the X-rays are absorbed by the battery casing which necessitates special cells with windows, neutrons have a penetration depth large enough to probe the entirety of cell. This has allowed measurements directly on commercial batteries, giving unique insights into the evolution of cell parameters and composition of the cathode and anode phase.

When measuring on commercial cells, contributions from all parts of the cell are observed which complicates the analysis of the diffraction data. A desire also exists to measure on non-commercial electrode materials prepared in the lab. Thus, there exists an incentive to develop a measuring cell which allows easy measurement on a variety of different cathode materials, either commercial or synthesized.

In this work, we present a new operando neutron diffraction battery cell, especially designed for the new beamline ErwiN at the FRM II research reactor at Garching, Germany. The cell uses a Zr/Ti-alloy with negligible scattering strength to eliminate contributions from the casing. We present data on the commercial cathode materials $LiFePO_4$ and $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ to demonstrate the capabilities of the cell, as well as on the non-commercial cathode material $LiNi_{0.5}Mn_{1.5}O_4$.

80

In-situ characterization at high temperature of VDM alloy 780 Premium

Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Johannes Munke (Department of Physics, Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Sebastian Mühlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Martin Bergner (Institut für Werkstoffe, Technische Universität Braunschweig), Bodo Gehrmann (VDM Metals International GmbH), Joachim Roesler (Institut für Werkstoffe, Technische Universität Braunschweig), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Ni-based superalloys are used for high temperature (T) applications that require good mechanical properties, as gas turbines. Among these alloy 718 is the most widely used with operation T up to 650 °C. In this alloy the austenitic matrix is strengthened by γ'l and γ'' precipitates. Other phases that can be formed are δ and η. The existence of the different phases, quantity and shape of the precipitates depend on composition, heat treatment and processing conditions. It is crucial to control their evolution with T in order to tailor the mechanical properties. The aim of increasing the operation T forces the development of materials stable at higher T. Waspaloy, with higher amount of γ', can be used at higher T but has a poor hot formability, while for the alloy 718Plus it is expected to have easier processing.
A new alloy called VDM 780 Premium, with good formability and the potential for high operation T, was selected for this investigation due to its direct industrial application. Measurements were performed on this alloy to determine its structure after different aging conditions. In-situ neutron diffraction (ND) and small-angle neutron scattering (SANS) experiments were carried out up to the dissolution temperature of all precipitates. We studied the amount of the phases present in the material and their stability with temperature as well as the evolution of cell parameters, grain sizes and morphologies as function of temperature.

81

An innovative testing machine for heating, quenching, tension, compression and cracking studies of industrial relevant high-temperature alloys – HiMat BMBF project

Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Johannes Munke (Department of Physics, Technical University of Munich), Frank Kümmel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Bodo Gehrmann (VDM Metals International GmbH), Steffen Neumeier (Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The development of new high temperature superalloys for aircraft engines and stationary gas turbines in power engineering requires higher service temperatures to enhance efficiency and reduce CO_2 emissions.
The development of these new materials require the structural (phase transformation) and mechanical (hardness) studies of strengthening and high temperature phases, precipitation kinetics (growth & dissolution), creep & crack growth and forging processes. This will include the development of a new testing machine for neutron scattering studies able to reproduce the rotation or forging forces at high T of a gas turbine which means tension and compression possibilities (up to 100 kN) and furnace heating (up to 1200 °C).
In the HiMat project, we will focus not only on the development of the testing machine but also on the study of different new high temperature superalloys:
- Fundamental studies (strengthening, phase stability…) on new developed Co-base superalloys (materials developed by FAU).
- Industrial studies (understanding of forging, creep resistance..) on VDM Ni-base superalloys (material developed by VDM Metals).

click here to go to
the poster list

82

Free thin film sample preparation for Users by Molecular Beam Epitaxy

**Sabine Pütter (Jülich Centre for Neutron Science (JCNS)
at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH)**

Patrick Schöffmann (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Thomas Brückel (Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI Quantum Materials and Collective Phenomena JCNS-2 / PGI-4, Forschungszentrum Jülich GmbH)

Molecular Beam Epitaxy (MBE) is a versatile tool to fabricate high quality and high purity epitaxial thin films with low intrinsic defect concentrations and atomic-layer control.
At the 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.
The MBE system is equipped with effusion cells, electron guns for electron-beam evaporation and a plasma source which may be run 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 films samples which are sensitive to ambient conditions are first fabricated in the MBE system and then measured at the neutron reflectometer MARIA of the JCNS utilizing a versatile small ultra high vacuum condition chamber. [1]
In our presentation we will give examples for high quality thin films like Fe_4N, $SrCoO_3$ or Nb/ Al_2O_3(1-1 0 2).
We are looking forward to discuss with you!

[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

83

Characterization of VDM Alloy 718 CTP (DIN 2.4668 / UNS N07718) in different hardened conditions and the relationship between hardening phases and the alloy's hydrogen embrittlement susceptibility

Julia Botinha (VDM Metals International GmbH)

Bodo Gehrmann (VDM Metals International GmbH), Helena Alves (VDM Metals International GmbH), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Johannes Munke (Department of Physics, Technical University of Munich), Artem Feoktystov (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH), Volodymyr Baran (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

The Nickel Alloy 718 was developed in the 60's for aerospace applications but due to its good corrosion resistance in sour gas application combined with the excellent strength properties, it found huge application in the Oil & Gas industry. Alloy 718 is a precipitation hardenable nickel-alloy enriched with amounts of niobium, molybdenum, titanium and aluminum, which combined grant the good properties.
The combination of nickel and aluminum drives to the precipitation of an ordered FCC Ni_3Al phase, Gamma'. When combined with niobium, an body-centered tetragonal Ni_3Nb phase precipitates, the Gamma''. Both precipitates are responsible for the strengthening of the austenitic Gamma matrix.
Studies have been carried out in order to compare and better understand the hydrogen embrittlement resistance of the three different aging conditions of Alloy 718 listed in the API 6ACRA. Different commercial heats were age hardened under the standard ageing temperature range defined by the API 6ACRA in order to produce material with minimum 120 ksi, 140 ksi and 150 ksi yeld strengths.
The interaction of H with the microstructure has been evaluated by means of Slow Strain Rate Tests under cathodic polarization in order to calculate the loss of elongation in the material after exposure to aggressive environment, what characterizes the suscepbility to hydrogem embrittlement. A structural characterization was made by means of neutron diffraction and small angle neutron scattering techniques.

84

SAPHiR: Neutron diffraction and high resolution radiography under high pressure and temperature conditions

Nicolas Walte (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Hans Keppler (Bayerisches Geoinstitut, Universität Bayreuth)

SAPHiR, the Six Anvil Press for High Pressure Radiography and Diffraction belongs to the suite of new instruments that are located in the Neutron Guide Hall East of FRM II. The aim of SAPHiR is to provide extreme pressure and temperature environments for polycrystalline samples, fluids, or melts. The pressure is generated by a three-axis multianvil press with a combined force of 2400 tons (24 MN), which currently generates pressures of up to 15 GPa in samples with volumes of 10-30 mm^3. Efforts are under way to increase the pressure to 25 GPa. Applications include phase transformations, reaction kinetics, crystallography of light-element-bearing high pressure phases, high resolution radiography, equations of state, and rheological studies. SAPHiR will use a thermal neutron beam that is focussed on the sample by an elliptic neutron guide. Due to geometrical restrictions by the multianvil press, neutron diffraction employs the time-of-flight method. The detector system combines four wave-length-shifting-fibre detector segments in the backscatter regime and three helium-3 detector banks at 90° from the incident beam and in the forward scatter regime. We are aiming for a diverse user community from materials science and geosciences, solid state physics, and chemistry. User access will commence once the infrastructure in the eastern neutron guide hall is completed, currently projected for 2021. Offline exploratory experiments can already be performed by interested research groups.

85

Optimising the γ/γ‘ microstructure and increasing the high temperature strength of a Co-base superalloy

Daniel Hausmann (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Cecilia Solis (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Lisa Freund (Friedrich-Alexander-Universität Erlangen-Nürnberg), Andre Heinemann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Mathias Göken (Friedrich-Alexander-Universität Erlangen- Nürnberg, Erlangen), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Steffen Neumeier (Friedrich-Alexander-Universität Erlangen- Nürnberg)

The newly developed polycrystalline Co-base-superalloy CoWAlloy2 ($Co_{41}Ni_{32}Cr_{12}Al_9W_5$ + Ti,Ta,Si,C,B,Zr,Hf) provides a high potential for application as wrought alloy due to the large gap between solidus and γ'-solvus temperature along with a high γ'-volume fraction. The scope of this study was the improvement of the high temperature strength by optimizing the γ/γ'-microstructure and adjusting different annealing steps.
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) at FRMII helped to understand the microstructural evolution during heat treatment. The size of the γ'-particles 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 gamma'-particle size, which can be explained by the weak and strong pair-coupling model of dislocations. A second annealing step leads to a further increase of yield strength due to an increasing γ'-fraction.

86

Phase transformations in CoRe-based alloys with Cr and Ni addition studied by in-situ neutron diffraction

Přemysl Beran (Nuclear Physics Institute of the CAS)

Debashis Mukherji (TU Braunschweig), Pavel Strunz (Nuclear Physics Institute of the CAS), Ralph Gilles (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Markus Hoelzel (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Joachim Roesler (Technische Universität Braunschweig, Institut für Werkstoffe)

Like other Co-based superalloys presently used in gas turbine static components, the Co-Re alloys use Cr to provide oxidation resistance [1]. Cr addition above 20 at.%, however, pose a challenge – namely the formation of topologically closed packed Cr_2Re_3-type σ-phase. It is generally avoided in high-temperature alloys as its presence causes brittleness. To improving oxidation resistance and, simultaneously, suppression of σ-phase, the alloys with a partial replacement of Cr by Ni are investigated. In-situ neutron diffraction measurements were performed during heating up to 1450°C and cooling for a various Ni (8, 15 and 25 at.%) and Cr (18 and 23 at.%) content alloys to study the allotropic transformation of the Co-matrix and the evolution of the low-temperature hexagonal and high-temperature cubic Co phases. Influence of the preparation technique to the initial phase composition was also investigated. The phase evolution was monitored, and an appearance of the secondary fcc phase [2] could be linked to the formation of the σ phase associated with a compositional change in the matrix. The σ-phase formation and its influence on the matrix phase separation – two fcc/hcp phases – in Co-Re-Cr-Ni alloys are an important discovery for the Co-Re alloy development and deserve further investigation.

[1] T. Depka, PhD thesis, Ruhr Universität Bochum, Germany, 2012.

[2] P. Beran, D. Mukherji, P. Strunz, R. Gilles, M. Hölzel, J. Rösler, Adv. Mat. Sci. Eng., 2018, 5410871

87

The multi-purpose three-axis spectrometer (TAS) MIRA at FRM II

Robert Georgii (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Markos Skoulatos (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Peter Böni (Department of Physics, Technical University of Munich)

The cold-neutron three-axis spectrometer MIRA is an instrument optimized for low-energy excitations. Its excellent intrinsic Q-resolution makes it ideal for studying incommensurate magnetic systems (elastic and inelastic). MIRA is at the forefront of using advanced neutron focusing optics such as elliptic guides, which enable the investigation of small samples under extreme conditions. Another advantage of MIRA is the modular assembly allowing for instrumental adaption to the needs of the experiment within a few hours. The development of new methods such as the spin-echo technique MIEZE is another important application at MIRA. Scientific topics include the investigation of complex inter-metallic alloys and spectroscopy on incommensurate magnetic structures.

88

Development of a new target station for external electric field application at PLEPS

Ricardo Helm (Universität der Bundeswehr München)

Werner Egger (Universität der Bundeswehr München), Marcel Dickmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Johannes Mitteneder (Universität der Bundeswehr München), Gotfried Kögel (Universität der Bundeswehr München), Peter Sperr (Universität der Bundeswehr München), Günther Dollinger (Universität der Bundeswehr München)

The Pulsed Low Energy Positron System (PLEPS) at the intense positron source NEPOMUC at the MLZ in Munich allows to measure positron lifetime spectra using a mono-energetic positron beam of variable energy between 0.5-20 keV. PLEPS is a unique tool to investigate open volume defects in a large variety of material systems, e.g. in wide bad-gap semiconductors or in thin layer structured semiconductors and insulators.
Defect identification in semiconductors and insulting materials is a challenging task, as one encounters a wide variety of different defect types, often with very similar positron lifetimes. To address this problem one possibility is to apply an external field to the sample and manipulate the positron diffusion after thermalization, thus driving the positrons to subtle structures i.e. thin layers, interfaces and internal surfaces. We present a newly designed target station which enables external field application and in situ measurement of voltages and currents during PALS measurements. With the three available power lines it is possible to apply voltages up to ±400V in different directions relativ to the sample surface and measure multiple electrical parameters at once.

89

Self-diffusion in Mercury investigated with quasi-elastic neutron scattering

Sandro Szabo (Heinz Maier-Leibnitz Center (MLZ) and Physics Department, Technical University of Munich)

Fan Yang (Deutsches Zentrum für Luft- und Raumfahrt), Winfried Petry (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Diffusion is a fundamental property of liquid with a high importance to many aspects in physics and material science. Despite its technical relevance it’s still not very well understood how atomic diffusion depends on properties, like the atomic mass, molar volume, and the melting point. The lack of internal degrees of freedom and the short-range, repulsive nature of metallic bonds make pure metals the closest analogy to a hard-sphere model system. Mercury has a rather high density and is the only metal, which is at room temperatures in the liquid state (Tl = 234 K). Hence, it is an ideal candidate to relate diffusion mechanisms over a wide temperature range when compared with other pure metals. We show QENS measurements of Mercury, carried out at the multi-disc chopper time-of-flight spectrometer TOFTOF at the research neutron source Heinz Maier-Leibnitz (FRM II). QENS probes atomic motion directly on a pico-second time scale, which allows reliable and precise in-situ observation of atomic transport processes on an absolute scale with rather small deviations. Thus, our QENS measurements can be compared with existing QENS data on metallic melts, which all exhibit considerable high melting points. This will contribute to a comprehensive understanding how atomic mass, molar volume, and the melting point affect the atomic motion of metallic melts.

90

Non-uniform capacity fading in lithium-ion batteries revealed by spatially-resolved diffraction of neutrons and synchrotron radiation

Dominik Petz (Department of Physics, Technical University of Munich)

Volodymyr Baran (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Michael Hofmann (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Martin Mühlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Cycling stability and capacity fading of Li-ion batteries are highly relevant for their application. A plenty of mechanisms directly leading to the capacity losses upon cycling are known, e.g. formation of passivation layers, losses of cyclable lithium etc. Typical Li-ion cells are characterized by non-uniform distributions of current, temperature and gradients in electrolyte and lithium concentrations, thus leading to heterogeneities in cell fatigue behavior. In the current contribution an example of non-uniform aging behavior will be shown based on the lithium-concentration in fully charged graphite anodes of cylinder-type Li-ion batteries with different number of cycles, which is directly correlated to the remaining capacity. Combined spatially-resolved diffraction studies unambiguously revealed development of heterogeneous Li distribution over the whole stripe of the negative electrode in charged state.

91

Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate $Li_{14}SiP_6$

Stefan Strangmüller (Department of Chemistry, Technical University of Munich)

Henrik Eickhoff (Department of Chemistry, Technical University of Munich), David Müller (Department of Chemistry, Technical University of Munich), Wilhelm Klein (Department of Chemistry, Technical University of Munich), Gabriele Raudaschl-Sieber (Department of Chemistry, Technical University of Munich), Holger Kirchhain (Department of Physicy, Augsburg University), Christian Sedlmeier (Department of Chemistry, Technical University of Munich), Volodymyr Baran (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Anatoliy Senyshyn (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Volker L. Deringer (Department of Chemistry, University of Cambridge), Leo van Wüllen (Department of Physicy, Augsburg University), Hubert A. Gasteiger (Department of Chemistry, Technical University of Munich), Thomas F. Fässler (Department of Chemistry, Technical University of Munich)

The development of all-solid-state batteries as high power and energy density storage devices has become one of the key challenges in solid-state chemistry and material science. Not only improvement of current electrode and electrolyte materials as well as the cell architecture, but also the search for new compounds is necessary to get access to a new generation of all-solid-state battery technology.
Recently, a new class of promising Li^+ conductors has been studied intensively. Lithium phosphidosilicates and -germanates offer, analogously to oxidosilicates, thiosilicates and thiophosphates, a large structural variety combined with decent Li^+ conductivity up to 10^{-4} S cm^{-1} at 25 °C.
Latest studies report on the preparation and characterization of the most lithium-rich phosphidosilicate $Li_{14}SiP_6$ revealing fast ionic conductivity of $\sigma > 10^{-3}$ S cm^{-1} at 25 °c. Characterization via X-ray diffraction (powder and single crystal) and elastic coherent neutron scattering experiments enabled the thorough investigation of the structural and thermal behavior of the compound. Activation energies, ionic and electronic conductivities have been determined using solid-state ^7Li NMR measurements as well as electrochemical impedance spectroscopy. Finally, diffusion pathways were analyzed by temperature-dependent powder neutron diffraction measurements in combination with MEM and DFT calculations to extend the knowledge about the material properties.

click here to go to
the poster list

92

Investigation of capacity fade mechanisms and modeling for lithium ion batteries cycled under different state of charge ranges

Jiangong Zhu (Karlsruher Institute of Technology (KIT))

Michael Knapp (Karlsruher Institute of Technology (KIT), IAM-ESS), Michael Heere (Karlsruher Institute of Technology (KIT)), Daniel Sørensen (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Haifeng Dai (Tongji University), Xuezhe Wei (Tongji University), Helmut Ehrenberg (Karlsruher Institute of Technology (KIT))

Regarding to that lithium-ion batteries are seldom used at the entire state of charge (SoC) interval for the vehicular usage conditions, investigating the battery fatigue mechanisms at different using SoC ranges could guide the battery management. 18650-type cells are cycled at various SoC intervals. In situ methods, e.g. differential voltage analysis (dV/dQ), neutron power diffraction (NPD), electrochemical impedance spectroscopy (EIS), are used to study the battery degradation mechanisms. The results indicate that high SoC range cycling (95%-75%, etc.) shows faster capacity degradation rates, low SoC range cycling (45%-5%, etc.) is more likely to have fatigue inconsistency and trigger the capacity drop. Cathode loss, anode loss, and loss of lithium ions are identified by dV/dQ for all cells at the end of life (700 cycles). The high SoC range cycling cells are investigated by NPD, and crystal structure parameters are observed. Two phases (NCA and NCM) in the cathode are identified, and the NCA is deemed to the main cathode loss by comparing their unit volume changes. EIS is employed to study the inconsistency of capacity fade at same cycling condition, indicating that the capacity fade dispersion deviation is mainly caused by accelerated lithium ion loss along with the ohmic resistance and solid electrolyte interphase resistance increase. At last, an empirical capacity fade modeling which is functional of SoC intervals and equivalent full cycles is proposed and verified.

93

On the use of $BaCe_{0.85}Y_{0.15}O_{3-d}$ as a multi-functional ingredient in solid oxide fuel cells

Kiril Krezhov (Institute of Electrochemistry and Energy Systems and Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences)

Daria Vladikova (Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences), Tanya Malakova (Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences), Gergana Raikova (Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences), Ivailo Genov (Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences)

Solid oxide fuel cells (SOFCs) offer a promising green technology of direct conversion of chemical energy of fuel into electricity. Barium cerates with Y-substitution at the Ce site, $BaCe_{1-x}YxO_{3-\delta}$, are well known for excellent conduction capabilities in the temperature range 400-800 °C as a result of the proton motion in the crystal lattice. We report on oxygen-deficient $BaCe_{0.85}Y_{0.15}O_{3-d}$ (BCY15) perovskites for which specialized impedance measurements discovered promising mixed ion (proton and oxide ion) conductivity at the intermediate operating temperatures. To realize a "monolithic design", which strongly simplifies the technology was proposed based on the introduction of a separate compartment (central membrane) for the water formation and evacuation. It has mixed ionic (proton and oxide ion) conductivity and porous structure since in O_2 flow BCY15 is an oxide ion conductor, in H_2 flow it is proton-conducting and in the central membrane, it is mixed ion-conducting. The characterization of the chemical composition and stability, oxygen stoichiometry and cationic ratios is known of great importance for understanding the defect-chemistry that would govern the transport properties. The structural details of powder, dense and porous samples of materials based on $BaCe_{0.85}Y_{0.15}O_{3-\delta}$ (BCY15) were investigated from full profile analysis of neutron and x-ray diffraction patterns. The materials operated satisfactorily as cathode, anode and central membrane in a test monolithic SOFC.

94

Size-dependent spatial magnetization profile of Manganese-Zinc ferrite nanoparticles

Mathias Bersweiler (Faculty of Science, Technology and Communication, University of Luxembourg)

Mathias Bersweiler (University of Luxembourg), P. Bender (Physics and Materials Science Research Unit, University of Luxembourg), L.G. Vivas ((Physics and Materials Science Research Unit, University of Luxembourg), M. Albino (Dipartimento di Chimica, Università degli Studi di Firenze), M. Petrecca (Dipartimento di Chimica, Università degli Studi di Firenze), Sebastian Mühlbauer (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), S. Erokhin (General Numerics Research Lab), D. Berkov (General Numerics Research Lab), C. Sangregorio (Dipartimento di Chimica, Università degli Studi di Firenze), Andreas Michels (Faculty of Science, Technology and Communication, University of Luxembourg)

In the present work, we report the results of an unpolarized small-angle neutron scattering (SANS) study on MZFO nanoparticles with the aim to elucidate the interplay between their particle size and the magnetization profile. Here, $Mn_{0.2}Zn_{0.2}Fe_{2.6}O_4$ nanoparticles covered with a thin layer of oleic acid (capping agent) were synthesized by co-precipitation or thermal decomposition. The chemical composition of the nanoparticles was determined using X-Ray Fluorescence (XRF). The studied MZFO nanoparticle samples have average diameters ranging from 8 to 80 nm according to TEM; XRD confirms in each case their single crystallinity. By taking advantage of the SANS technique, we demonstrate that the smallest nanoparticle are homogeneously magnetized. However, with increasing particle size we observe the transition from uniform to nonuniform magnetization states. Field-dependent results for the pair-distance distribution function p(r) on a 38-nm-sized specimen reveal that the internal spin disorder can be suppressed by an increasing field. The experimental SANS data are supported by the results of micromagnetic simulations, which confirm an increasing inhomogeneity of the magnetization profile of the particle with increasing size. The results presented demonstrate the unique ability of SANS to detect even very small deviations of the magnetization state from the homogeneous one.

This work was supported by the financial support of the EU Horizon-2020 project “AMPHIBIAN” (720853).

95

NREX – polarized neutron/X-ray reflectometer

Yury Khaydukov (Max-Planck Institute for Solid State Research)

Franz Tralmer (Max Planck Institute for Solid State Research, Thomas Keller (Max Planck Institute for Solid State Research), Bernhard Keimer (Max Planck Institute for Solid State Research)

The high resolution/polarization 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/GIND horizontally as well as vertically for specular and diffuse scattering measurements. Neutrons are detected with a 20 x 20 cm² 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. Results of several experiments recently measured at NREX are shown.

click here to go to the poster list

NICOS - The instrument control user interface

96

Jens Krüger (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

NICOS Developer Team

NICOS (Networked Instrument COntrol System) is the general user interface to control the instruments at the MLZ. NICOS is now in use at 23 instruments.
A number of standard commands exist, and instrument specific commands are possible. Python is also used as the command and scripting language.
There is a script execution component, components to create a history of measured data as well as of nearly all parameters of the instrument, various option to display the current measured data (detector image, scan data, and so on).
To display the status of the instrument and current measurement the most important instrument and measurement parameters may be displayed on a screen or via an internet browser.
A newly developed protocol for sample environment integration (SECoP) is available as well as the plug-and-play integration of decoupled embedded systems (e.g. sample environment systems)
Nearly all components are written in Python which gives a high degree of platform independence (Linux, Windows, macOS). It also allows easy implementation of new features (devices, commands, data sinks, and GUI components).
An international collaboration with the SINQ at PSI and the ESS has started.

Combined Neutron and Gamma Tomography at the NECTAR instrument

97

Adrian Losko (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Dominik Bausenwein (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Thomas Bücherl (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Burkhard Schillinger (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich) Michael Schulz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Rudolf Schütz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

NECTAR is a superior 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, gamma rays are produced in the same process. The production of these gamma rays is inevitable as they are inherent with the production of fission neutrons and the principles of collimating or stopping them. 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. Here we present the advantages of combining the information gained from neutron imaging in conjunction with gamma imaging at the NECTAR beam-line, providing novel characterization capabilities.

click here to go to
the poster list

98

POWTEX – Angular- and Wavelength Dispersive, High-Intensity Neutron TOF Diffractometer

Yannick Meinerzhagen (Institute for Inorganic Chemistry, RWTH Aachen)

Andreas Houben (Institute for Inorganic Chemistry, RWTH Aachen), Philipp Jacobs (Institute for Inorganic Chemistry, RWTH Aachen), Werner Schweika (Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH), Thomas Brückel (Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI Quantum Materials and Collective Phenomena JCNS-2 / PGI-4, Forschungszentrum Jülich GmbH), Richard Dronskowski (RWTH Aachen)

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 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 ^{10}B 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 ^{10}B is a development for POWTEX that achieves high efficiency for a remarkably large coverage of nine steradians with almost no blind spots. For powder samples, 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 B_0. 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 powder data (intensity as function of 2θ and λ).

99

The Coincident Doppler-Broadening Spectrometer at NEPOMUC

Vassily Vadimovitch Burwitz (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Leon Chryssos (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Lucian Mathes (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Thomas Schmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich), Christoph Hugenschmidt (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Doppler broadening-spectroscopy (DBS) of the 511keV gamma line, generated by positron-electron-annihilation, provides information on lattice defects, sensitive to concentrations as low as $1e^{-7}$ vacancies per atom. In addition the chemical surroundings of defects can be analyzed by coincident DBS (CDBS). The CDB-Spectrometer at the Neutron-induced Positron Source Munich (NEPOMUC) is presented. Ongoing improvement works will be shown.
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 ≈ 300 µm (FWHM) beam spot and high resolution measurements with a micro beam with a 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 four 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 T dependent defect spectroscopy, iii) a cryostat with T_{min}=40 K and iv) a device for in situ tensile tests.
Ongoing improvements comprise: an automated beam optimization system and an increase in the number of detectors combined with an upgrade of the readout electronics.

click here to go to
the poster list

100

99

Monitoring selectivity of gold cluster growth/formation on antifouling-relevant zwitterionic thin block copolymer coatings

Apostolos Vagias (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich)

Simon Schaper (Department of Physics, Technical University of Munich), Lucas Kreuzer (Department of Physics, Technical University of Munich), Wei Chen (Department of Physics, Technical University of Munich), Suzhe Liang (Department of Physics, Technical University of Munich), Marc Gensch (Deutsches Elektronen-Synchrotron (DESY)), Pallavi Pandit (Deutsches Elektronen-Synchrotron (DESY)), Matthias Schwartzkopf (Deutsches Elektronen-Synchrotron (DESY)), Stephan Roth (Deutsches Elektronen-Synchrotron (DESY)), Jonas Drewes (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), Niko Carstens (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft),Thomas Strunskus (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), Franz Faupel (Christian-Abrecht-Universität zu Kiel (CAU), Institut für Materialwissenschaft), André Laschewsky (Institut für Chemie, Universität Potsdam, and Fraunhofer-Institut für Angewandte Polymerforschung), Peter Mueller-Buschbaum (Heinz Maier-Leibnitz Zentrum (MLZ) and Department of Physics, Technical University of Munich)

Polysulfobetaine (PSB) films serve as promising antifouling coatings [1]. In addition, metal-coated thin polymer films hold also tremendous potential for antifouling and antibacterial applications [2]. However, the exact limit to how much one may tune antifouling by means of altering the block copolymer nanostructure with a metal sputtered on top of the polymer remains practically unexplored. Schwartzkopf et al. [3] have shown that sputtered gold can exhibit wetting selectivity with different affinities in each constituent of a PS-b-PEO block copolymer film. The correlation between gold growth and affinity to the particular polymer phase of the PSB copolymer structure and its impact on antifouling efficiency remain elusive. By in-situ microfocus GISAXS (μGISAXS) we present the nanostructure evolution of gold film growth on thin (<100 nm) polymer films. We compare poly (N-isopropyl methacrylamide) (PNIPMAM) homopolymer, PNIPMAM-b-PSB diblock copolymer and a PSB homopolymer. We inspect for potential selectivities during gold sputtering on these polymer films and potential correlation between polymer-metal nanocomposite structure to antifouling efficiency.

[1] A. Laschewsky, A. Rosenhahn, Langmuir 35 (5), 1056 (2019)

[2] J. Ren, P. Han, H. Wei and L. Jia, ACS Appl. Mater.Interfaces 6, 3829 (2014)

[3] M. Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017)