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Book of Abstracts

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Plenary session I / **3**

Welcome

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Plenary session I / **4**

Fundamental Physics

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Plenary session I / **5**

Detectors for neutron scattering applications

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Plenary session II / **43**

Introduction to Soft Matter

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Soft materials are characterized by both, complexity and flexibility, where structure is often defined in terms of time scales. In particular, the spontaneous association (self-assembly) process of their molecules into a 3-D geometry can be expanded to the control of more complex nanometer-scale functional systems. Areas of interest encompass phase separation and self-assembly of block copolymers and metal-polymer nanocomposites in thin film geometry, as well as nanomaterials for energy related applications. Some examples of thermodynamic and kinetic driven interfacial self-assembly processes will be discussed. Structural/property investigations using a diverse range of experimental techniques such as small- and wide angle X-ray/neutron scattering methods, electron and atomic force microscopy, as well as optical, electrical and magnetic analyses will be presented.

Plenary session II / **7**

Moderated brainstorming: Optimisation of internal MLZ processes

Quantum phenomena / **28**

Under-compensation effect in the Kondo insulator (Yb,Tm)B12

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We present an inelastic neutron scattering study of the influence of isoelectronic Tm substitution on the low-energy structure and temperature dependence of the dynamical magnetic response in (Yb,Tm)B12 solid solutions. Substantial changes have been observed in the spectral structure and temperature evolution of the Yb contribution to the inelastic response for a rather low content of magnetic Tm ions. The spin-exciton-like resonance mode near 15 meV is steeply suppressed at the lowest measured Tm concentration (x = 0.08). The spin gap is replaced by a pseudogap at concentrations lower than 0.15. These results point to a specific effect of impurities carrying a magnetic moment (Tm, as compared to Lu or Zr) in a Kondo insulator, which is thought to reflect the "under-compensation"of Yb magnetic moments, originally screened in pure YbB12. A parallel is made with the strong effect of Tm substitution on the temperature dependence of the Seebeck coefficient in (Yb,Tm)B12.

Material Science / **36**

Recent Positron Beam Experiments at NEPOMUC

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In solid state physics and surface science the positron is applied as a highly mobile nano-probe for the detection of vacancy-like defects and their chemical surrounding in a non-destructive way. Positron lifetime measurements with pulsed beams allow the identification of different types of vacancies. Benefitting from the elemental sensitivity and selectivity of the positron, buried metallic layers and clusters can be investigated by coincident Doppler broadening spectroscopy of the annihilation line. Within this contribution the basic properties of positron annihilation studies will be briefly explained. The benefit of positron beam experiments will be elucidated by selected experiments, such as defect sensitive positron lifetime experiments and the elemental selective (coincident) Doppler broadening spectroscopy.

Material Science / **40**

Investigation of the surface of binary metallic alloys using Positron annihilation induced Auger Electron Spectroscopy, XPS and STM

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The characterization of the elemental composition of surfaces is of high importance for the understanding of many surface-related processes such as catalysis or oxidation.
Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental omposition of only the topmost atomic layer of a specimen. The positron beam facility NEPOMUC delivers a high intensity positron beam of 10^9 e+/s and enables measurement times of only a few minutes per PAES spectrum. Thus, time-dependent PAES is possible and enables the in-situ observation of surface kinetics. The upgraded surface spectrometer at NEPOMUC uses the complementary techniques PAES, XPS and STM for a comprehensive surface analysis.

Financial support by the BMBF (project no. 05K13WO1) is gratefully acknowledged.

Quantum phenomena / **14**

Structural transition between disordered vortex solids

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Small-angle neutron scattering reveals the presence of an ordered vortex solid phase in high quality optimally doped single crystalline (Ba1-xKx)Fe2As2. Vortex solid Bragg peaks are not described by the Bragg glass prediction. Simultaneously, the vortex solid structure factor shows a sharp drop as function of magnetic field, that is correlated with the second peak feature in isothermal hysteresis loops. Hence, the vortex order-disorder transition in this material is unrelated to the presence of vortex solid dislocations.

Soft matter / **21**

Reorientation of microdomains in cylinder forming diblock copolymer thin films during solvent vapor annealing: simulations with dissipative particle dynamics

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Solvent vapor annealing (SVA) is an efficient technique to refine and control the structure of ordered block copolymer films, promising as functional templates for nanolithography and membrane preparation. SVA was simulated in the case of intermediate A/B block segregation and fast solvent evaporation. Under these conditions, the domain orientation is controlled by the solvent selectivity. If the solvent preferentially dissolves the short blocks, lying cylinders in thermodynamic equilibrium appear. In contrast, solvents selective for the long blocks reorient the cylindrical domains along the solvent concentration gradient, i.e. vertically. This may be explained by the Gibbs-Marangoni effect and by the interplay of adsorption of the short and the long blocks at the two film interfaces. Longer film drying, attained after strong initial film swelling in a moderately good solvent, produces the most ordered films. The mechanism of the film evolution is discussed in detail.

Material Science / **49**

IN-BEAM NEUTRON ACTIVATION ANALYSIS AT MLZ

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Prompt gamma activation analysis (PGAA) at MLZ has been successfully applied for the analyses of a large variety of samples even with masses less than a milligram, as well as for the investigation of low-cross-section nuclides and radioactive targets. Recently, a low-background counting chamber has been installed next to the PGAA instrument thus enabling the counting of induced radioactivity. Since the flux is almost as high as that in smaller reactors (6E10 cm^-2 s^-1), it can efficiently be used for traditional neutron activation analysis. PGAA and NAA complement each other, the first one provides the matrix composition, while the second one the trace elements, however their common potential has just partly been explored.
Liquid-scintillation counting of nuclides emitting charged particles induced by cold neutrons has been tested, too. The objective of this development is to increase the sensitivity of in-beam analysis for lithium, boron, and nitrogen.

Quantum phenomena / **51**

Investigation of magnetic ground states of pyrochlore iridate and hafnate by polarized neutron scattering

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Pyrochlore iridates and hafnates A2B2O7 (A= rare earth ion, B=Ir, Hf), in which both the A site and the B site consists of corner-shared tetrahedral, are of particular interest due to the presence of both strong spin-orbital coupling and geometrical frustration. Recently, we have successfully synthesized high quality powder samples of Nd2Ir2O7 and Nd2Hf2O7 which high quality powder samples have been synthesized by solid-state reaction. By employing polarized neutron spectrometer DNS, we

have investigated these two compounds magnetic ground states. Both two samples show k=0 antiferromagnetic long-range ordering but with different ordering temperature which may be caused by the magnetic ordering of Ir4+ ions.

Soft matter / **17**

Stimuli-responsive reversible hydrogels from triblock polyampholytes and terpolymers

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The mechanical properties of hydrogels formed by block copolymers with charged blocks are very sensitive to pH value. Using small-angle neutron scattering, we have investigated the structures of a triblock polyampholyte having negatively and positively charged blocks in dependence on the pH value and salt content. pH variation alters the charge densities of the ionizable blocks and thus the charge asymmetry. At low charge asymmetry, the chains collapse into large globular structures, whereas at higher charge asymmetry, a network is formed [1]. Salt addition makes the hydrogel softer due to a gradual disintegration of the network. Another system under study is a terpolymer with glassy end blocks and a middle block containing both positively and negatively charged monomers. Their relative amounts in dependence on pH lead to gross changes in the correlation between the micelles.
[1] M. Dyakonova et al., Macromolecules 47, 7561 (2014).

Quantum phenomena / **12**

TISANE @ SANS-1, Perspectives and ideas

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We present the implementation of the time resolved stroboscopic small angle neutron scattering technique TISANE at the SANS-1 instrument at MLZ. TISANE is based on the cyclic perturbation of the sample where the time-dependent response is measured. By means of a chopper system, a microsecond time-resolution can be achieved. We discuss existing applications and possible future perspectives for experiments using TIANE.

Material Science / **55**

in situ SANS - a new method to non-destructively investigate lithiation processes in pouchbag type batteries

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We report on our measurements with the SANS-1 instrument at Heinz Maier-Leibnitz Zentrum (MLZ), Garching. In-operando small-angle neutron scattering data of NMC||Separator||Graphite cells was collected during a complete charging and discharging cycle. In addition single battery components were measured separately to distinguish the various component signals.
The in-operando data shows a variation of the integrated total scattering intensity in dependence of the transferred charge. The curve features are directly associated with the lithiation process of the cathode or anode materials. Work on modelling these lithiation kinetics as observed by SANS and correlating them with other techniques is in progress.

Soft matter / 16

Aggregation behavior of doubly thermo-responsive poly(sulfobetaine-b-(N-isopropylmethacrylamide) diblock copolymers

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Diblock copolymers consisting of a thermo-responsive poly(N-isopropylmethacrylamide) (PNIPMAM block) and a zwitterionic poly(sulfobetaine) (PSB block) feature both a lower and an upper critical solution temperature (LCST and UCST) in aqueous solution. P(SB-b-NIPMAM) expected to form in water the following phases: (i) micelles with PNIPMAM shell and PSB core or vice versa at low and high temperatures and unimers and (ii) large aggregates in the intermediate temperature range, depending on the chemical structure and the molecular mass of the PSB block as well as on the presence of electrolyte.

The aggregation behavior in D2O with dual stimuli (temperature and electrolyte concentration) is studied by temperature-resolved small-angle X-ray and neutron scattering (SAXS, SANS). We have found that the aggregation of P(SB-b-NIPMAM) in D2O occurs above LCST and below UCST and that the structure depends on the blocks lengths, whereas the salt-induced structural changes were only minor.

Material Science / 41

Characterization of High Purity Ni(100)-foils for Positron Moderation in a Novel Positron Microbeam Setup

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The positron beam facility NEPOMUC at the FRM II provides a mono-energetic positron beam with an intensity of 10^9 moderated e+/s. The CDB spectrometer at NEPOMUC enables depth dependent and spatially resolved defect studies by using conventional doppler broadening spectroscopy(DBS), and element-specific measurements with coincident DBS. For depth dependent measurements, the positron implantation energy can be adjusted from 0.5 to 30 keV. The lateral resolution amounts to 300 um.
For the development of a positron micro beam with a diameter of <5 um a 100 nm thick Ni(100) remoderation foil will be installed in transmission geometry to increase the beam brightness. To achieve a high yield of re-emitted moderated positrons, the Ni foil has to be annealed and surface contaminations such as carbon and oxygen have to be removed. Therefore, temperature-dependent XPS and DBS measurements were performed for characterizing the surface contaminations and for determining the annealing behaviour.

Quantum phenomena / **37**

Gracing incidence small angle neutron scattering of incommensurate magnetic structures in MnSi thin films

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The topological stability of skyrmions in bulk samples of MnSi and the observation of spin transfer torque effects at ultra-low current densities have generated great interest in skyrmions in chiral magnets as a new route towards next generation spintronics devices. Yet, the formation of skyrmions in MBE grown thin films of MnSi reported in the literature is highly controversial. We report gracing incidence small angle neutron scattering (GISANS) of the magnetic order in selected thin films of MnSi grown by state of the art MBE techniques. In combination with polarised neutron reflectometry (PNR) and magnetisation measurements of the same samples our data provide direct reciprocal space information of the incommensurate magnetic order, clarifying the nature of magnetic phase diagram.

Quantum phenomena / **79**

Band structure of helimagnons in MnSi resolved by inelastic neutron scattering

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A magnetic helix realizes a one-dimensional magnetic crystal with a period given by the pitch length. Its spin-wave excitations –the helimagnons –experience Bragg scattering off this periodicity leading to gaps in the spectrum that inhibit their propagation along the pitch direction defined by the

wavevector. Using high-resolution inelastic neutron scattering the resulting band structure of helimagnons was resolved by preparing a single crystal of MnSi in a single magnetic-helix domain. At least five helimagnon bands could be identified that cover the crossover from flat bands at low energies with helimagnons basically localized along the pitch direction to dispersing bands at higher energies. In the low-energy limit, we find the helimagnon spectrum to be determined by a universal, parameter-free theory. Taking into account corrections to this low-energy theory, quantitative agreement is obtained in the entire energy range studied with the help of a single fitting parameter.

Poster Session / **25**

Structuring of thin films for application in organic photovoltaics

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Organic photovoltaics using thin polymer films to convert light to electric energy are gaining interest as a promising alternative to conventional solar cells. Potential advantages include low-cost production processes, material availability and device flexibility, but power conversion efficiencies are still comparatively low. Several methods have been described to enhance the cell performance, among them the utilization of high-efficiency materials as well as nano- and microstructuring methods. We combine both strategies, using model low band gap systems and structuring techniques like nano-imprint lithography (NIL) to enhance the charge carrier separation and performance of the active layer. The optical properties of active layer thin films are investigated using UV/Vis and PL measurements. Morphological studies include optical microscopy, AFM and X-ray diffraction methods.

Poster Session / **23**

Laser-ablated nanoparticles for hybrid photovoltaics

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Hybrid solar cells of inorganic and organic materials mark an important class of next generation solar cells, since they combine the advantages of inorganic materials, such as high stability, with the advantages of organic materials, such as tailoring of band gaps and potential low cost production.

We introduce laser-ablated nanoparticles into hybrid solar cells. The production of functionalized TiO2 nanoparticles via laser ablation in liquid is achieved with two approaches, using a TiO2 particle

suspension as target and a solid titanium target [1]. The crystallinity of the active layer is investigated with X-ray diffraction (XRD) and grazing incidence wide angle X-ray scattering (GIWAXS). The hybrid solar cells show high fill factors and open circuit voltages underlining the potential of the novel material and the environment-friendly processing method.

[1] Körstgens et al., Nanoscale 9, 2900 (2015).

Poster Session / **42**

On the morphology of PCPDTBT:PC71BM thin blend films for organic photovoltaics

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The use of solvent additives provides a route to strongly improve the performance of polymer:fullerene based organic solar cells (OSC). In case of PCPDTBT:PC71BM, the use of 1,8-octanedthiol (ODT) has been reported to boost the power conversion efficiency from 2.8% to 5.5%. However, the physical mechanism of this improvement, as well as the impact on degradation behavior, when ODT is used is not yet fully understood. In the present work, we illuminate how ODT affects the nanometer scaled morphology of thin PCPDTBT:PC71BM thin films. Using grazing incidence small and wide angle X-ray scattering methods, and optical spectroscopy, ODT is found to enhance polymer crystallization and phase separation on a nanometer scale. The formation of a fullerene rich topping layer is observed by X-ray reflectivity. When ODT is used, the influence of blend composition is lost. This knowledge paves the pathway for studying the degradation behavior of PCPDTBT based solar cells.

Poster Session / **34**

Efficiency increase of P3HT:PCBM organic solar cells doped with iron oxide(II,III) nanoparticles

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Organic solar cells of P3HTPCBM have received the highest attention due to easy commercial availability. In the present work P3HT:PCBM bulk heterojunction solar cells are doped with different concentrations of surface coated Fe3O4 nanoparticles. At low nanoparticle concentrations (below 1 wt%) an increase in the power conversion efficiency (PCE) of up to 11% is found. This improvement in the device performance cannot be related to changes in the film morphology or in the film crystallinity, according to grazing incidence small and wide angle x-ray scattering experiments. Instead, an increase in the effective exciton lifetime is accounted as origin of the efficiency increase.

Poster Session / **22**

Characterization of PTB7-Th:PC71BM bulk heterojunction solar cells: influence of blend ratio

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Organic photovoltaic devices are a promising source of green energy. In such cells the generated excitons are separated by the electric field built up by the difference in work functions at the interfaces between the polymer (PTB7-Th) and the fullerene (PC71BM). Thus, a crucial parameter for solar cell performance is the morphology of the polymer-rich (or fullerene-rich) domains.
The ratio between the two materials has been varied and the optical properties of resulting films have been characterized via UV-Vis absorption and photoluminescence. The surface morphology has been investigated with AFM and optical microscope. The inner film morphology has been examined by GISAXS. Additionally, the vertical material composition has been inspected via X-rays reflectivity and a deeper sight into the crystalline structure via GIWAXS. Finally, the solar cells performances have been tested via current-voltage characterization and external quantum efficiency (EQE).

Poster Session / **29**

Maghemite nanoparticles embedded in thin block copolymer films

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Maghemite nanoparticles (NPs) embedded inside a polymer tem plate mark a novel class of hybrid materials which have attracted high interest due to the potential for many applications such as sensors and magnetic storage mediums. The control of the alignment of the maghemite NPs within the

polymer NPs is essential for making well-aligned highly-oriented metal oxide-polymer nanocomposites. The alignment of NPs in polystyrene-b-poly(N-isopropylacrylamide) P(S-b-NIPAM) diblock copolymer (DBC) films is studied. The structure of the resulting films is studied at different concentrations of NPs using SEM, AFM, and GISAXS. The results present a morphological transition from parallel cylinders to perpendicular cylinders with incorporation of NPs into the DBC films. At high NP concentration, large particles aggregates are formed on top of the polymer surface. The magnetic properties of the nanocomposite films at different temperatures are measured and compared with theoretical predictions.

Poster Session / 24

Morphology of Polymer-Metal Interfaces

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Within recent years, metalized polymer films have attracted increasing interest due to their possible applications in organic electronic devices. In these devices, a thin metal layer is used as an electric contact in conjunction with an active layer comprising a semiconducting polymer. Since, the electronic properties of such contacts are influenced by the interface between the metal and the polymer, a precise control of the metal growth on top of the organic material is required.
In the presented work, we investigate the growth kinetics of aluminum on top of poly(3-hexylthiophene) (P3HT) by in-situ grazing incidence small angle x-ray scattering (GISAXS) for different molecular weights of the polymer. Hereby, the growth process is monitored in real-time and temporal information on structural parameters of the deposited material can be extracted. We complement the study with different imaging, optical and electronic characterization methods.

Poster Session / 26

In-situ investigation of Aluminum metal sputtering on nanostructured PS-b-P3HT diblock copolymer thin films

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Thin metal coatings on polymers are widely used in electronic devices, such as organic photovoltaic devices and organic field effect transistors. The morphology of the metal electrode on the polymer

film plays a crucial role in the performance of such devices. An aluminum contact on polystyrene-b-poly(3-hexylthiophene) (PS-b-P3HT) is prepared with DC sputter deposition. Growth and morphology are monitored using GISAXS and XRR. The nano- and microstructure of the sputtered films is also investigated using OM, AFM and SEM. The crystallinity of P3HT block of the diblock copolymer is examined using GIWAXS. Up-right cylinder structure of P3HT is obtained due to micro-phase separation. The Al layer shows correlated roughness which changes with sputter time, showing a growth on the copolymer film. The observed structures are discussed in the framework of selective decoration of Al on a particular domain.

Poster Session / **27**

Spray deposited ZnO scattering layers for OLED applications

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White organic light-emitting diodes (WOLEDs) hold high potential for room lighting, display technology and beyond. By using specific phosphors the internal quantum efficiency of OLEDs reaches values close to 1 but the overall efficiency is still reduced by insufficient photon extraction. A common way to overcome this lack of efficiency is the insertion of scattering centers to the device. Among the different material systems, nanostructured metal oxide layer holds high potential because of their high stability and their high refractive index. In this work zinc acetate dihydrate was used in combination with a structure giving diblock copolymer template and sol-gel chemistry to obtain a processable solution for ZnO deposition. To achieve a reasonable film thickness the produced solution was deposited on glass substrates by spray coating. The film morphology as probed by x-ray scattering techniques and SEM is related to the spectral response to gain a structure-function relationship.

Poster Session / **20**

Characterization of the optical and morphological properties of high-efficiency polymers

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Organic photovoltaics are gaining impact as a feasible alternative to conventional solar cells. Using polymers as active material has several potential advantages, for instance reduced production costs and an increased device flexibility. However, efficiencies of polymer solar cells stay far below those of inorganic photovoltaics. In order to enhance the solar cell performance, recent research efforts focus on identifying highl-efficiency polymers. This has led to the development of low band gap materials with efficiencies approaching 10 %. Our work focuses on a group of high-efficiency polymers

called PBDTTTs. We investigate the optical and morphological properties of model systems using the prominent examples PTB7 and PTB7-Th. Applied characterization techniques include UV/Vis measurements, optical microscopy, AFM, XRR, XRD and GISAXS/GIWAXS. Exploratory solar cells link the power conversion efficiency to parameters such as the active layer composition and morphology.

Poster Session / **46**

Drug Carriers based on HPMA Nanoparticles: Molar Mass and Buffer Type

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A promising way to achieve site-specific delivery of anticancer agents is to use the enhanced permeation and retention (EPR) effect of N-(2-hydroxypropyl) methacrylamide (HPMA) nanoparticles containing the drug doxorubicin (Dox) [1]. The present research in this field focuses on exploration of the particle structure and tuning of their properties. A low critical micelle concentration (CMC) and particle sizes in the range of 1-100 nm are of importance.

The aim of the present study is to investigate the influence of molar mass of the HPMA backbone with randomly distributed cholesterol moieties. Moreover, diblock copolymers from pure HPMA and HPMA with cholesterol are investigated with a focus on their CMC. Using fluorescence correlation spectroscopy (FCS) and small-angle neutron scattering (SANS), the CMC as well as the size and structure of the nanoparticles are determined in a phosphate buffer.

[1] Filippov, S.K. et al., Biomacromolecules 14, 4061 (2013).

Poster Session / **44**

Foam-like structure of titania films via spray coating for photovoltaic application

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Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics. Controlling the pore size is crucial for photovoltaic applications, such as in case of dye-sensitized solar cells (DSSCs) and solid state DSSCs. In this study, spray coating is used, which is deposition method allowing for scaling-up to large scale production. A sol-gel process is used to form the nanostructured titania films. The structural evolution of the

films was probed by in situ grazing incidence small angle X-ray scattering (in situ GISAXS) on the nanoscale during the spray process. The morphology of the sprayed films is characterized with scanning electron microscopy (SEM) and optical microscopy. The pore size can be controlled from 5.7 to 10.5 nm by changing the recipe of the sol-gel solution as well as by the details of the applied spray circles.

Poster Session / 45

A Fluorescence Life-time Study of the Drug Delivery System Based on HPMA Copolymers

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Polymer drug carriers based on HPMA copolymers have been studied extensively over the past few years [1,2], to understand the behavior and shape of the copolymers in dilute solutions. However, there is a lack of knowledge on the behavior of these drug carriers in real human blood environment. We use HPMA copolymers labeled with fluorescent dyes, which are dissolved in a solution of human serum albumin (HSA). This facilitates the determination of their size by fluorescence life-time correlation spectroscopy (FLCS). Compared with FCS, a separate autocorrelation function is calculated in FLCS for each fluorescent component determined by its life-time, which enables an easier separation of different contributions.
[1] S. K. Filippov, et al., Biomacromolecules, 2012, 13 (8), 2594–2604
[1] S. K. Filippov, et al., Biomacromolecules, 2013, 14 (11), 4061–4070

Poster Session / 32

Spray Deposition of Titania Films with Incorporated Crystalline Nanoparticles for All-solid-state Dye-Sensitized Solar Cells Using P3HT

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Spray coating has received immense attention for the film deposition because it is simple, low cost, and usable for large-scale production. In the present work, this technique is employed to fabricate titania films for solid-state dye-sensitized solar cells (ssDSSCs) which use solid-state hole-transporting

materials (HTM) for dye regeneration and hole transport. ssDSSCs, consisting of organic HTM and n-type inorganic nanocrystals, are of great interest due to the combined advantages of both organic and inorganic components. We investigate this kind of solar cells fabricated using mesoporous titania films as electron transporting materials, a metal-free dye D149 as a light harvester, and P3HT as HTM. For optimizing the device performance, we introduce crystalline titania nanoparticles into the titania film in order to obtain a more effective titania photoanode. The morphology and crystallinity of titania films are investigated, showing a crucial influence on final device performance.

Poster Session / 18

Investigating the morphology of MAPbI3-xClx highly efficient perovskite solar cells

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Perovskite solar cells offer the opportunity of easy and potentially cheap processing techniques very comparable to other next generation solar cell such as organic and dye-sensitized solar cells. In addition, the optimization of preparation routines has led to power conversion efficiencies (PCE) of over 15 % for solution processed devices. Device performance, however, is strongly linked to film morphology which in turn depends on the applied preparation protocol.
In our present work we have prepared perovskite thin films with an established 2-step synthesis method. We have investigated precursor and perovskite film with GISAXS and observe a strong correlation of lateral crystal sizes before and after conversion which we attribute to constrained crystal growth. Additionally, we find an accumulation of smaller crystals within the film in contrast to the surface.

Poster Session / 39

Hybrid polymer-metal oxide based membranes for lithium ion micro batteries

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In the light of an increasing demand on power sources for portable electronic devices, the nano-scaled lithium based membranes paves the way for new opportunities regarding design, application and integration of rechargeable batteries. In this work, the morphology of lithium ion-polymer hybrid material based on high-molecular-weight polystyrene-block-polyethylene oxide PS-b-PEO

diblock copolymers at different temperatures and salt concentrations is investigated. The use of block copolymers enables the formation of conductive lithium containing polyethylene oxide (PEO) domains as well as mechanically stable glassy polystyrene (PS) domains. The tendency of the PEO block to crystallize is highly suppressed with increasing both, the salt doping level and the temperature. Further incorporation of small semiconductor nanoparticles is investigated. As indicated from SAXS measurements, the PEO chains change from a compact conformation to an amorphous conformation upon metal oxide upload.

Poster Session / **38**

Crystallinity and phase separation in nanocomposite copolymer electrolytes for Lithium batteries

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Long scale transition to green energy and wide penetration of electric cars, demand for batteries with high power density, and good mechanical stability. The electrolyte is of crucial importance for both. Poly(ethylene oxide) (PEO), although very reliable, has two drawbacks: 1) poor mechanical stability 2) crystallinity, acting as barrier to the ion mobility. Mechanical stability may be provided by copolymerization with polystyrene (PS) and introduction of nanoparticles, which in addition are known to suppress crystallinity. We blended silica nanoparticles into an electrolyte consisting of a PS-PEO diblock copolymer and LiTFSI salt. In this first stage of our work we study by X-ray scattering and DSC the effects of nanoparticles on phase separation and crystallinity: a salt loading of molar ratio Li:EO = 0.1 already eliminates PEO crystallinity, and a moderate loading of nanoparticles (~1wt%) enhances the thickness of the PEO lamellae, which may lead to increased conductivity.

Poster Session / **72**

Li-diffusion pathway in the structure of Al-substituted LiTi2(PO4)3

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Due to reaching the stability limit for organic solvents in liquid electrolytes the research on Li-ion batteries adopting solid lithium electrolyte (all-solid-state) becomes of increasing relevance. Among various inorganic solid state lithium conductors the NASICON type compounds are the most promising, where Al-substituted LiTi2(PO4)3 - Li1.3Al0.3Ti1.7(PO4)3 possesses one of the highest ionic conductivities (~10-3 S/cm).
Investigation of series of Al-substituted LiTi2(PO4)3 was carried out. Elastic coherent neutron scattering experiments were performed on the powder diffractometer SPODI at the neutron source FRM II and on the D2B diffractometer at the ILL. Powder diffraction data were collected at room temperature and at fixed temperatures in the range of 100-800 °C (with increment of 100 °C) upon heating. Analysis of the Li positions in the structure as well as the estimation of possible Li-diffusion pathways was performed.

Poster Session / 30

Hybrid thermoelectrics based on polymer-nanoparticle composites

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Thermoelectrics present a promising alternative to conventional solar cell technology energy generation. A temperature gradient applied along the thermoelectric material induces an electrical voltage, which is transformed into electrical power.
Although thermoelectrics have already reached high conversion efficiencies, limited and expensive raw materials and cost- and energy-intensive processing have limited the widespread application.
Therefore, we investigate the possibilites of using conductive polymers, processed with standard thin film fabrication methods like spin-coating, and the influence of introduced nanoparticles on the thermoelectric properties. Polymers show several advantages regarding availability, environmental aspects and facile fabrication into thin films. The promising electrical properties of the polymer blend PEDOT:PSS has been heavily investigated in literature. We mix silicon nanoparticles into the film and investigate the properties of the hybrid film.

Poster Session / 35

degradation in printed polymer:fullerene thin films for organic photovoltaics

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In comparison to conventional silicon solar cells, organic photovoltaics (OPVs) offer several advantages, like ease of production and a high versatility. Nevertheless, their lifetime needs to be prolonged, so that a profitable large-scale production becomes feasible. Therefore a detailed understanding of the degradation mechanisms is necessary. In our investigations, the degradation of OPVs is investigated by means of atomic force microscopy (AFM), X-ray reflectivity (XRR), UV/Visible light spectroscopy (UV/Vis) and photoluminescence spectroscopy (PL). We address UV induced aging of P3HT:PCBM active layers, printed in a positive shim mask slot dye coater. The possibility of printing OPVs enables large-scale fabrication, in contrast to other production methods, like spin-coating. A lot of research has already been done with OPVs produced by spin-coating. However, it is not clear how the method of film application affects the aging behavior.

Poster Session / 19

The morphology of perovskite solar cells

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In recent years lead halide perovskites, especially those based on methylammonium lead iodide (MAPbI3), have attracted increasing attention as a new solar cell material due to a rapid increase in the power conversion efficiency (PCE) from 3.9% in 2009 to 20.1% in 2015 for solar cells fabricated with MAPbI3 as the active layer. Despite the quick increase in PCE the relationship between preparation method, film morphology and solar cell performance is still not fully understood.
We probe this relationship by combining XRD and GIWAXS to investigating the morphology of perovskite thin films prepared by a variety of different methods. We correlate our findings to the photovoltaic performance of solar cells fabricated by these techniques with the aim of establishing a link between film morphology and device performance.

Poster Session / 47

Collapse behavior of a thermo- and pH-responsive block copolymer in water

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Orthogonally switchable block copolymers show rich phase behavior in aqueous solution. In dependence on temperature and pH, e.g. unimers, core-shell micelles, reverse core-shell micelles or large aggregates may be formed. We investigate a block copolymer with a polybasic pH sensitive block of (diisopropylamino)ethyl methacrylate and a thermoresponsive block composed by a random copolymer of (methoxyethoxy)ethylmethacrylate and oligo(ethylene glycol)methyl ether methacrylate featuring a lower critical solution temperature (LCST)[1]. Micelles will present a core of one or the other block, depending on whether the temperature and pH values are below or above the LCST and the pKa.

The critical micelle concentrations and the micellar hydrodynamic radii are determined by temperature-resolved fluorescence correlation spectroscopy. The structures of the micelles and the aggregates are assessed by small-angle X-ray scattering.

[1] Alves, S. P. C. et al. J. Phys. Chem. B 118, 3192 (2014).

Poster Session / 31

Energy-level alignment at hybrid interfaces between ZnO and organic semiconductors

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Designing hybrid inorganic-organic semiconductor devices requires control over the energy-level alignment at the hybrid interface to achieve desired functionality such as efficient charge-carrier transfer. In this study, the energy-level alignment of the interface between Zn-terminated ZnO (0001) and the hole transport material N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (alpha-NPD) p-doped with the strong electron acceptor 2,2'-(perfluoronaphthalene-2,6-diylidene)dimalononitrile (F6TCNNQ) is investigated. It is shown that F6TCNNQ can be used to control the energy-level alignment of both, the inorganic and the organic semiconductor. Using photoelectron and optical absorption spectroscopy, it is identified that F6TCNNQ on the ex situ annealed ZnO induces surface band bending and increases the work function by up to 1.6 eV and that F6TCNNQ undergoes integer charge transfer with alpha-NPD.

Plenary session III / **73**

Overview on Superconductivity Research in Quantum Phenomena Group

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Superconductivity is one of the most fascinating phenomena in condensed matter since its macroscopic behavior is apparently originated from the quantum mechanics of electrons: Formation of electron pairs that are bound together via a small attractive interaction between them, also called Cooper pairs. Over several decades, dedicated theoretical works revealed that collective motions of either atoms or spins, which are precisely measurable physical quantity via neutron scattering, are the most important ingredient for Cooper pairing. In this talk, I will introduce how the neutron scattering study contributes to the superconductivity research field by presenting a few recent example cases from Quantum Phenomena group at MLZ.

Plenary session III / **9**

Moderated brainstorming: Improving the user structure of MLZ

Fuel development / **81**

High density fuel development and core conversion at FRM II

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FRM II's nuclear license contains an obligation to exchange its nuclear fuel to a lower enrichment once such a fuel is available. This task contains essentially two major pillars, the participation in the world-wide efforts to develop the fuel and to perform the necessary core calculations for this specific reactor. In the last 10 years, a scenario for the core conversion has been developed and significant progress has been made in fuel manufacturing and irradiation behaviour understanding. This talk will overview these developments and also argues on the associated boundary conditions and difficulties.

Plenary session II / **64**

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Plenary session II / **65**

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Plenary session II / **66**

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Plenary session II / **67**

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Plenary session II / **68**

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Plenary session II / **76**

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Plenary session II / **77**

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Plenary session II / **78**

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Towards a High Brilliance Neutron Source

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Research with neutrons in Europe is undergoing severe changes. While several medium flux research reactors have been decommissioned, construction of the world's most powerful pulsed spallation source has started in Lund. At JCNS we are considering several alternative routes where the entire chain from particle source through particle accelerator, target, moderator, reflector, shielding, beam extraction, beam transport all the way to the detector is being optimized. We are exploring the limits of accelerator or laser driven neutron sources based on nuclear reactions in the lower MeV regime. Although fewer neutrons are being produced per incident particle, such a source is significantly cheaper than a spallation source and allows a better coupling of target-to-moderator and moderator-to-beam transport system. Of particular importance is the optimization of the moderator.

Softmatter II / **52**

Change of Fractal Dimension during the early stages of Lysozyme Crystallization

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In this study we focussed on the question of how to grow crystals as large as possible in light of their use as samples for neutron protein crystallography. We investigated the early stages of the crystallisation process where the directions are set between the growth of many small crystals or few large ones. We used lysozyme since it is considered as a model system for crystal growth. Small angle neutron scattering was used in combination with static light scattering in order to realize an extended q-range. In situ dynamic light scattering at the neutron scattering sample cell was used to obtain an overview of all sizes present in the crystallisation process. We could observe a fractal growth of the crystal seeds with a change in the fractal dimension from 1.0 to 1.7 in the first 90 min. This can be interpreted that at first a branched crystal seed is formed which grows more in a linearly. Later, the space between the arms is filled to cross over to a more densely packed fractal.

Material Science / 48

Hydrogen dynamics in β-$Mg(BH_4)_2$ in the picosecond timescale

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Among the complex hydrides, magnesium borohydride is attractive due to a quite good thermodynamic stability and high hydrogen storage capacity (14.9 H2 wt %). Quasielastic neutron scattering (QENS) has been performed beta phase of Mg(11BH4)2 at the cold neutron time-of-flight spectrometer TOFTOF at FRM II, Munich. Spectra were reordered in the range of temperature from 11 to 500 K, in order to investigate the [BH4] unit dynamics. At low temperature a strong inelastic contribution has been observed, whereas at higher temperatures the quasielastic contribution is predominating. A jump rotation dynamic has been identified, superimposed to a vibrational dynamic of the entire [BH4] units. The quasielastic signal, as well as the vibrational signal, have been evaluated and used to determine the hydrogen motion in the scanned range of temperature and in the picoseconds time scale.

PhD students / 59

Talk 1

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Structure / **57**

Homogeneity of lithium distribution in cylinder-type Li-ion batteries

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Spatially-resolved in situ neutron powder diffraction with gauge volume 2x2x20 mm3 has been applied to probe the lithium concentration in the graphite anode of four different Li-ion cells of 18650-type in charged state. Information about underlying processes defining lithium distribution is crucial for the manufacturing of safe, robust and high-performance Li-ion cells. Structural studies performed in combination with electrochemical measurements and X-ray computed tomography under real cell operating conditions unambiguously revealed non-homogeneity of lithium distribution in the negative electrode. Deviations from a homogeneous behaviour have been found in both radial and axial directions of 18650-type cells and were attributed to effects involving cell geometry and electrical connection of electrodes, which might play a crucial role in the homogeneity of the lithium distribution in the active materials within each electrode.

PhD students / **60**

Talk 2

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PhD students / **61**

Talk 3

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Talk 4

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Material Science / **56**

Stability and growth of TaC precipitates in Co-Re superalloys for ultra high temperature applications studied by in-situ SANS

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Co-Re alloys are being developed in order to supplement Ni-base superalloys in future gas turbines for ultra-high temperature applications. The complex interplay between the different existing mesoscopic phases could be studied in-situ at high temperatures. It was shown that the amount and distribution of the stabilizing mono-carbide of TaC phase strongly depends on the stoichiometry of alloyed components. The stability of a fine distribution of TaC in the CoRe matrix could be shown at temperatures up to 1300℃. Currently, the effect of different heat treatments is under investigation and in-situ SANS and microscopic studies show long-term stability of very small (< 80 nm) TaC precipitates. Additionally, it was possible to observe time resolved phase transformations of large precipitates (~100 nm) in-situ with a time resolution of 10 seconds. This method makes it possible to observe fast changes in the particle size with any associated change in volume fraction.

Structure / **13**

Hot single crystal neutron diffraction on HEIDI - an overview

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For about 10 years the single crystal diffractiometer HEIDI (operated by RWTH Aachen for JCNS) provides user groups from around the world valuable information about the chemical or magnetic structures of their samples. These detailed structural data are an important basis for those groups to gain successfully new insights into their scientific topics.
The presentation contains an overview of the instrument and various interesting results from the field of solid state physics, chemistry and mineralogy.

Softmatter II / **33**

Nanocomposites composed of HEUR polymer and magnetite iron oxide nanoparticles: Structure and dynamics

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We study nanocomposites consisting of a polymer matrix which consists of hydrophobically modified ethoxylated urethane polymers (HEUR) with embedded coated magnetite nanoparticles. Two different kinds of coatings are compared namely the hydrophobic coating, composed of oleic acid and oleylamine, and the hydrophilic coating composed of a cationic surfactant, C18TAB, as an additional layer to the hydrophobic magnetic nanoparticles. We focused on the structural characterization through small angle neutron scattering (SANS) measurements of such nanocomposites in two different morphologies: as thin dry films and as hydrogels. We also performed magnetic response measurements on the nanocomposites in the dried state. In order to have information about the dynamics, and both electrical and mechanical properties of the nanocomposites in the dried state, we performed dielectric spectroscopy measurements.

PhD students / **63**

Talk 5

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Material Science / **53**

In-Situ Neutron Reflectometry during Thin Film Growth by Sputter Deposition

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While the structural characterisation of thin films during growth by various in-situ techniques is common practice, the in-situ measurement of the magnetic properties of films using (polarized) neutron reflectometry is a challenging task. Within a collaboration of TUM, Uni Augsburg and MPI Stuttgart, we operate a mobile sputtering facility for the growth and in-situ monitoring of magnetic multilayers. In our contribution, the setup and polarized in-situ neutron reflectivity measurements on in-situ grown Fe/Cr carried out at the ToF reflectometer REFSANS at the FRM II neutron source and at the AMOR beamline at PSI will be presented. At the latter, use of the Selene neutron optical concept allows very fast polarised neutron reflectivity measurements to be performed within only 15min per spin direction, allowing for un-contaminated surfaces in the coating process. As further example, induced magnetism in Pd/Fe/Pd heterostructures, observed using this method, will be presented.

Structure / **74**

Neutron Laue diffraction at MLZ

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First neutron Laue experiment was performed in the year 1947 by E. O. Wollan, C. G. Shull and M. C. Marney [1]. You can easily perform it at home every beamtube at MLZ. You just need salt, indium plate and photographic film. Put everything in given order to the beam and wait few second. Process the film and look to the picture. You get information about your crystal quality, orientation, symmetry, crystal structure, magnetic structure, impurities···Or just use new nLaue instrument at

SR8b beamport, right after the RESI instrument.
The first part of this talk will be devoted to the introduction to Laue technique and its pros and cons. After that I will show you what type of data you can obtain and how to treat it with the open source software Esmeralda [2].
[1] E. O. Wollan, C. G. Shull, and M. C. Marney, Phys. Rev. 73 (1948) 527
[2] http://lauesuite.com

Softmatter II / **50**

Octanol-Water Partition Coefficient: Fact or Fiction

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In pharmaceutical sciences, determining the partition coefficient P of a drug is a must, as this quantifies the drug solubility and distribution in the body. P is defined as the ratio of a drug concentration in a mixture of two immiscible phases, usually octanol and water. It implies that the two phases are structurally unaffected by the drug. SAXS reveals that octanol, as well as octanol in equilibrium with water, is structured, having polar groups that form a mesophase. Introducing drugs of different hydrophobicity changes the regularly packed water nanodroplets in the hydrated octanol mesophase. It is also possible for certain drugs to bring and keep more water into octanol by expanding the droplets into freely diffusing aqueous lacunae. We have proved that drugs do not partition into a homogeneous octanol, but mainly binds to a responsive octanol-water mesophase, which is heterogeneous. One should consequently reinterpret the P data in terms of octanol-water binding constants.

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Softmatter II / **80**

MSca - multiple scattering simulation for backscattering spectrometers

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We have developed a simulation package ‘MSca’ to provide an analysis tool for multiple scattering effects in backscattering spectrometers such as SPHERES. Multiple scattering has non-trivial wavevector and

energy transfer dependency and is thus difficult to tackle by analytical methods only. Also, due to the geometry of backscattering instruments, there are additional multiple scattering channels not present in, for example, time-of-flight instruments. In this talk an introduction to 'MSca', the simulation procedure, and some examples of the effects of multiple scattering will be given.

Material Science / **54**

Characterizing novel anode materials for Li-ion batteries using TOF-GISANS

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Titania nanotube arrays are an interesting alternative anode material for use in Li-ion batteries due to their excellent cycling stability and enhanced safety compared to graphite. Moreover when such nanotube arrays are used as support for a thin silicon film, the resulting composite material has the additional advantage of a high lithium storage capacity. We present a detailed comparison of the morphology of such self-organised conductive TiO2 nanotube arrays, with and without silicon coating, using TOF-GISANS technique. We obtain a prominent lateral correlation of the TiO2 nanotubes of ~ 94 nm and an inner nanotube radius of ~ 46 nm. The porosity averaged over the entire film is extracted to be 49%. The nanotube radius is reduced to half (~23 nm) through the silicon coating, but the prominent lateral structure is preserved. Such in-depth morphological investigations over large sample volumes are useful towards development of more efficient battery electrode morphologies.

Plenary session IV / **75**

In situ Neutron Diffraction of martensitic Ni-Ti Shape Memory Alloys

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Ni-Ti shape memory alloys are used for medical and engineering applications with increasing commercial success. Despite their technological importance, the elastic behaviour of the monoclinic B19' martensite phase remains elusive, because martensite single crystals are not available for mechanical testing. DFT calculations have provided a monoclinic angle of $\gamma \approx 107^\circ$ instead of $\gamma \approx 98.5^\circ$, as we observe experimentally. In the present work we performed in situ neutron diffraction on a B19' Ni-Ti sample applying tensile load. A special load frame was used where the sample and load axis can be rotated in an Eulerian cradle. This technique allows to separate the effects of elastic and inelastic deformation processes.

Plenary session IV / **11**

Material Science

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In situ Neutron Diffraction of martensitic Ni-Ti Shape Memory Alloys

Ni-Ti shape memory alloys (SMAs) are used for medical and engineering applications with increasing commercial success. Despite their technological importance, the elastic behaviour of the monoclinic B19'martensite phase remains elusive, because martensite single crystals are not available for mechanical testing. DFT calculations have provided elastic constants for 0 K involving a monoclinic angle of $\gamma \approx 107^\circ$ [1] instead of $\gamma \approx 98.5^\circ$, as we observe experimentally. In recent experimental work 5 out of 13 independent elastic constants were calculated [2].
In the present work we performed in situ neutron diffraction on a B19' Ni-Ti sample (Mf≈44℃) applying tensile load. A special load frame was used where the sample and load axis can be rotated in an Eulerian cradle. This technique allows to separate the effects of elastic and inelastic (detwinning) deformation processes.
Evaluation of previous neutron experiments indicated complex behavior with changes from constant-strain to constant-stress microstructures during loading to 4% pseudoplastic strain. In our recent experiment diffractograms were recorded in the elastic regime at ~0.2, ~0.4 and ~0.6% strain allowing to isolate the orientation dependent elastic strain of the B19'structure from textural changes (caused by variant reorientation). Applying micromechanical models we can then calculate the single crystal elastic-constant-tensor of Ni-Ti B19'.