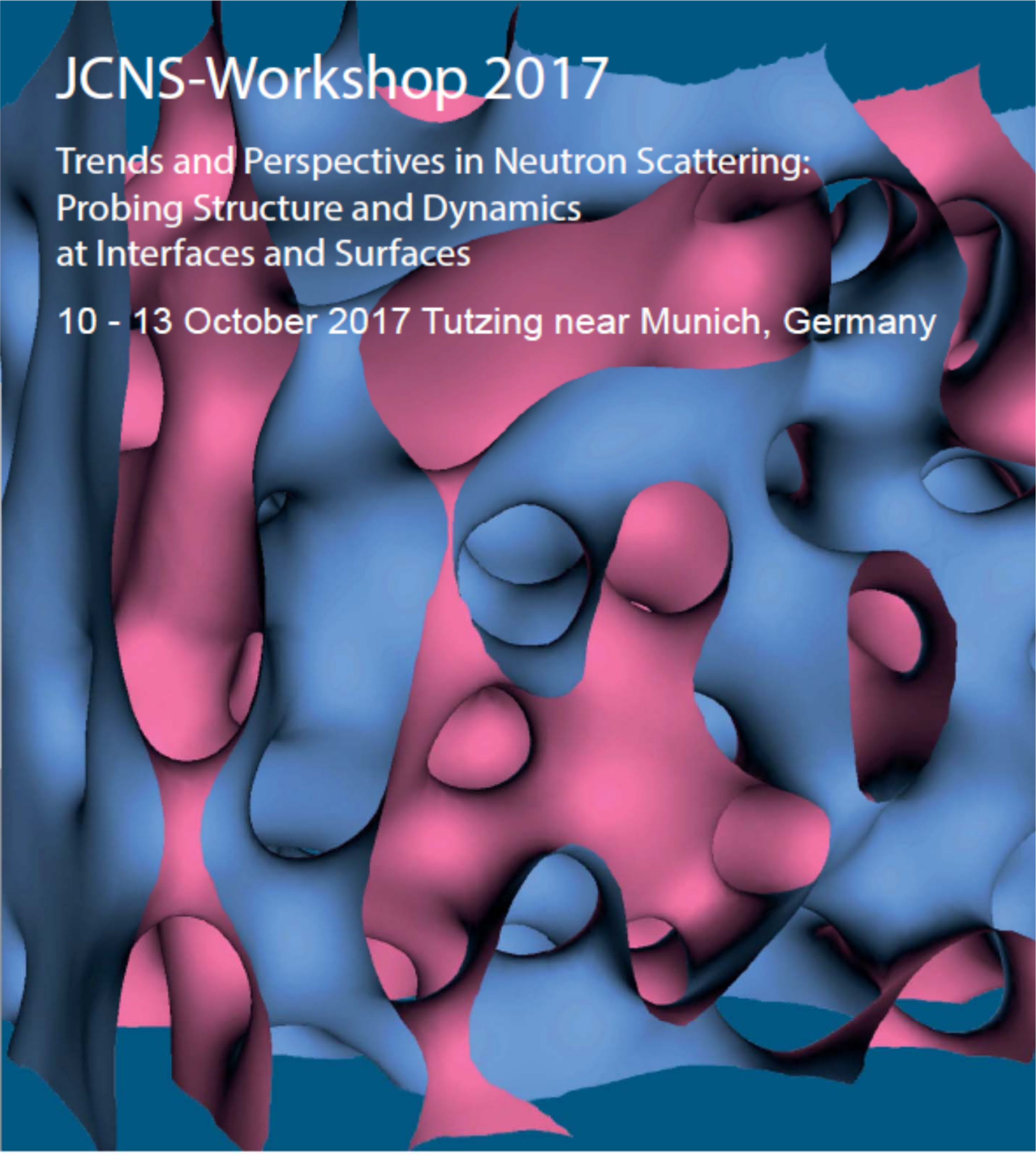

JCNS-Workshop 2017

Trends and Perspectives in Neutron Scattering: Probing Structure and Dynamics at Interfaces and Surfaces

10 - 13 October 2017 Tutzing near Munich, Germany

Member of the Helmholtz Association

Abstract booklet

Jülich Centre for Neutron Science

JÜLICH FORSCHUNGSZENTRUM

MLZ Heinz Maier-Leibnitz Zentrum

Welcome to the JCNS Workshop 2017

Dear colleagues,

Evolution of structure and composition at interfaces between materials affects a large variety of intrinsic and functional parameters defining interaction and reaction schemes. The analytical techniques capable of exploring the interfaces are still very limited, and more often only ex situ studies are performed. Neutron techniques are capable of operando studies of interfaces, of visualization of buried interfaces and interactions and of probing interfacial kinetics and dynamics. They have become an extensively growing field of research.

The JCNS Workshop 2017 held in Tutzing, Germany on 10-13 October, 2017, aims at highlighting recent approaches and developing ideas on the adaptation of neutron reflectometry, small angle neutron scattering, neutron spectroscopy, neutron imaging and depth profiling and neutron spin echo spectroscopy.

The workshop will discuss current requirements and developments in probing surfaces and interfaces using such techniques. In particular the workshop is devoted to novel and upcoming experimental opportunities with various new instruments in operation or planned at neutron facilities to discuss the scientific options and capabilities in this area.

The workshop is organized by the Jülich Centre for Neutron Science (JCNS) of the Forschungszentrum Jülich.

The organizers like to thank all partcipants and hope you all will enjoy a interesting conference.

Thomas Brückel Thomas Gutberlet

JCNS Workshop 2017 - Program

	Tu. 10. Oct. 2017	Wen. 11. Oct. 2017	Th. 12. Oct. 2017	Fr. 13. Oct. 2017
	Registration	**Buried Interfaces**	**Interfacial and Surface Dynamics**	**Magnetic Interfaces**
09:00-09:30		**Adrian Rennie**	**Regine von Klitzing**	**Sean Langridge**
09:30-10:00		**Ali Zarbakhsh**	**Stefan Wellert**	**Valeria Lauter**
10:00-10:15		Victor Petrenko	Reiner Zorn	Dieter Lott
10:15-10:45		Coffee Break	Coffee Break	Coffeee Break
		Magnetic Nanoparticles	**Interfacial and Surface Dynamics**	**Soft and Biological Surfaces and Interfaces**
10:45-11:00		**Andreas Michels**	Lucas Kreuzer	Tobias Widmann
11:00-11:15			Tetyana Kyrey	Chris Garvey
11:15-11:30		Dominique Dresen	Sebastian Jaksch	Jarek Majewsky
11:30-11:45		Elisabeth Josten	**Peter Müller Buschbaum**	Leonardo Chiappisi
11:45-12:00		Asmaa Qdemat		
12:00-13:00		**Lunch**	Lunch	Lunch
	Magnetic Surfaces	**Novel Instrumentation**	**Modelling and Instrumentation**	End of Workshop
13:00-13:15	**Björgvin Hjörvarson**	**Robert Cubitt**	Brian Maranville	
13:15-13:30			Gennady Pospelov	
13:30-13:45	**Mike Fitzsimmons**	Andrew Jackson	Stefano Pasini	
13:45-14:00		Olaf Holderer	Amir Syed Mohd	
14:00-14:15	Sergey Kozhevnikov	Artur Glavic	Matthias Kühnhammer	
14:15-14:30	Wolfgang Kreuzpaintner	Henrich Frielinghaus	Jean-Francois Moulin	
14:30-15:00	Coffee Break	Coffee Break	Coffee Break	
	Soft and Biological Surfaces and Interfaces	**Novel Instrumentation**	Excursion	
15:00-15:15	**Tommy Nylander**	Sabine Pütter		
15:15-15:30		Yury Khaydukov		
15:30-15:45	**Maikel Rheinstaedter**	Peter Konik		
15.45-16:00		Egor Vezhlev		
16:00-16:15	Alexandros Koutsioumpas	Peter Falus		
16:15-16:30	Franz Adlmann			
16:30-18:00	Poster Session	Poster Session		
	A. Feoktystov, A. Glavic, E. Kentzinger, V.I. Petrenko, P. Schöffmann, A. Stellhorn, A. Sarkar, X. Senlin, M. Waschk, M. Wolff, M. Zamponi			
19:00-21:00			Workshop Dinner	

Abstracts

Oral and poster presentations

Tu. 10. Oct. 2017		
09:00-12:00	Registration	
12:00-13:00	Lunch	
	Magnetic Surfaces	
13:00-13:30	**Björgvin Hjörvarson**	Emergent magnetic order: Artificial spin ice structures
13:30-14:00	**Mike Fitzsimmons**	Applications of polarized neutron scattering to guide development of novel functional heterostructures
14:00-14:15	Sergey Kozhevnikov	Neutron Zeeman beam-splitting for the investigations of magnetic nanostructures
14:15-14:30	Wolfgang Kreuzpaintner	Polarised Neutron Reflectometry Applied to In-Situ Thin Film Growth
14:30-15:00	Coffee Break	
	Soft and Biological Surfaces and Interfaces	
15:00-15:30	**Tommy Nylander**	Neutron scattering techniques reveals the structure and dynamics lipid non-lamellar phases at the solid/liquid interface
15:30-16:00	**Maikel Rheinstaedter**	Molecular membrane biophysics
16:00-16:15	Alexandros Koutsioumpas	Elucidating lipid membrane spreading on surfaces by time-resolved neutron reflectivity
16:15-16:30	Franz Adlmann	Depth resolved GISANS from liquid solid interfaces
16:15-18:00	Poster Session I	A. Feoktystov A. Glavic E. Kentzinger S. Mattauch V.I. Petrenko A. Sarkar P. Schöffmann A. Stellhorn A. Sarkar M. Waschk M. Wolff S. Xia M. Zamponi

Wen. 11. Oct. 2017		
	Buried Interfaces	
09:00-09:30	**Adrian Rennie**	Using GISANS and Reflection to Understand the Structure of Colloidal Dispersions near Interfaces
09:30-10:00	**Ali Zarbakhsh**	Polarised neutron Reflectivity and the Magic Angle Tuning of the Contrast
10:00-10:15	Victor Petrenko	Operando neutron reflectometry study of lithium enriched deposition on metal electrode in contact with liquid electrolyte
10:15-10:45	Coffee Break	
	Magnetic Nanoparticles	
10:45-11:15	**Andreas Michels**	Magnetic SANS as a probe to disclose internal interfaces
11:15-11:30	Dominique Dresen	Magnetic structure of ferrite nanoparticles on a square lattice
11:30-11:45	Elisabeth Joosten	Magnetic nanoparticles
11:45-12:00	Asmaa Qdemat	The spin structure of highly ordered arrangement of magnetic nanoparticles
12:00-13:00	Lunch	
	Novel Instrumentation	
13:00-13:30	**Robert Cubitt**	Advances in Neutron Reflectometry Techniques: Coherent Summing and Refractive encoding
13:30-13:45	Andrew Jackson	Opportunites in Surface Scattering at the European Spallation Source
13:45-14:00	Olaf Holderer	The neutron spin echo spectrometer J-NSE: the past and the future
14:00-14:15	Artur Glavic	Reflectometers at the European Spallation Source
14:15-14:30	Henrich Frielinghaus	Instrumental developments for grazing incidence neutron scattering experiments for nano-scale tribology studies
14:30-15:00	Coffee Break	
	Novel Instrumentation	
15:00-15:15	Sabine Pütter	Aside from neutron instruments: thin film fabrication by molecular beam epitaxy at the Jülich Centre for Neutron Science
15:15-15:30	Yury Khaydukov	Probing magnetic dynamics at interfaces using waveguide PNR
15:30-15:45	Peter Konik	Octagonal neutron guide for the horizontal sample reflectometers
15:45-16:00	Egor Vezhlev	Neutron Depth Profiling at a focused neutron beam to study Li-ion transport in thin-film batteries
16:00-16:15	Peter Falus	WASP Wide Angle SPin echo instrument for spectroscopy not just on surfaces

16:15-18:00	Poster Session II	A. Feoktystov A. Glavic E. Kentzinger S. Mattauch V.I. Petrenko A. Sarkar P. Schöffmann A. Stellhorn A. Sarkar M. Waschk M. Wolff S. Xia M. Zamponi

Th. 12. Oct. 2017		
	Interfacial and Surface Dynamics	
09:00-09:30	**Regine von Klitzing**	Neutron Scattering for Studying Structure and Dynamics of Stimuli Sensitive Polymer Coatings
09:30-10:00	**Stefan Wellert**	Near surface dynamics of adsorbed and tethered polymer systems: Results and instrumental aspects
10:00-10:15	Reiner Zorn	Description of poly(ethylenepropylene) confined in nanopores by a modified Rouse model
10:15-10:45	Coffee Break	
10:45-11:00	Lucas Kreuzer	In-situ time of flight neutron reflectometry study of the swelling and exchange kinetics of multi-stimuli responsive PNIPAM based block copolymers
11:00-11:15	Tetyana Kyrey	Inner structure and dynamics of the stimuli-responsive polymer microgel particles adsorbed on surface
11:15-11:30	Sebastian Jaksch	Nanorheology: Using neutrons to discover the dynamics of biological membranes
11:30-12:00	**Peter Müller Buschbaum**	Probing thin film nanostructures generated by block copolymer self-assembly using advanced scattering techniques
12:00-13:00	Lunch	
	Modelling and Instrumentation	
13:00-13:15	Brian Maranville	Instrument operations for the CANDOR reflectometer: handling and reducing data, modes of operation and current construction status
13:15-13:30	Gennady Pospelov	BornAgain: simulation and fitting framework for nuclear and magnetic GISANS
13:30-13:45	Stefano Pasini	Magnetic field-shape optimization and new superconducting coils for the high-resolution neutron spin-echo spectrometer (J-NSE) at MLZ

13:45-14:00	Amir Syed Mohd	Connecting MARIA with the MBE system: Polarized Neutron Reflectivity of thin Co films in UHV conditions using portable transport chamber
14:00-14:15	Matthias Kühnhammer	Development of a foam cell for SANS measurements in the framework of a modular sample environment system
14:15-14:30	Jean-Francois Moulin	Fitting Reflectometry Data Revisited
14:30-15:00	Coffee Break	
15:00-19:00 19:00-21:00	Exkursion Workshop Dinner	

Fr. 13. Oct. 2017		
	Magnetic Interfaces	
09:00-09:30	**Sean Langridge**	Revealing the nanoscale and interfacial behavior in complex magnetic systems at the ISIS spallation neutron source: current capabilities and future opportunities
09:30-10:00	**Valeria Lauter**	Peculiarities of Time-of-Flight Grazing Incidence Neutron Scattering with Polarized Neutrons
10:00-10:15	Dieter Lott	Chirality effects in Rare-Earth Multilayers investigated by the analysis of full polarized neutron reflectometry maps
10:15-10:45	Coffee Break	
	Soft and Biological Surfaces and Interfaces	
10:45-11:00	Tobias Widmann	Swelling and exchange kinetics in PNIPAM microgel thin films probed with in-situ neutron reflectometry
11:00-11:15	Chris Garvey	Small molecule profiles between lipid bilayers by neutron diffraction
11:15-11:30	Jarek Majewsky	Neutron scattering investigations of bio-interfaces: from model lipid membranes to living cells
11:30-11:45	Leonardo Chiappisi	A simple, single-step procedure for the preparation of responsive surfactant-polysaccharide multilayered coatings
11:45-12:00		
12:00-13:00	Lunch	
	End of Workshop	

Tuesday 10.10.17, 13:00-13:30

Emergent magnetic order: Artificial spin ice structures

Björgvin Hjörvarsson

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Patterning magnetic structures is a mean of engineering additional energy scales into magnetic materials. The resulting properties can be unique and strongly deviating form the parent material, as e.g. exemplified by the formation of artificial spin ice structures from permalloy films [1]. Despite much progress in elucidating the properties of such arrays, the `spins' in the systems have only recently been shown to exhibit phase transitions and dynamic response [2-5]. The criteria for obtaining phase transitions will be discussed and exemplified.

The spin dimensionality of the mesospins is determined by the aspect ratio of the islands. For example, an elongated islands can be described as Ising like[2], while circular islands can behave as XY like, in the absence of crystalline anisotropy [6].

A phase transition of two dimensional Ising like mesospins, forming artificial spin ice structures will be demonstrated [2,4]. The use of patterned structures opens up completely new ways of designing magnetic metamaterials, for example, it is possible to make structures with mesospins having different spin dimensionality [6]. An example of a designed master-slave like influence will be shown and how XY slaves can be used as an interaction modifier in Ising like mesospins.

The results clearly demonstrate the possibility to design new energy and length-scales in materials, giving rise to new and intricate properties. The nature of the emergent order is only rudimentarily explored and coupling between different physical properties are still unknown. The role of scattering experiments will be dwelled upon, with emphasis on the possible role of off-specular scattering, allowing new way of addressing phase transitions and fluctuations in this new type of metamaterials.

[1] Artificial 'spin ice' in a geometrically frustrated lattice of nanoscale ferromagnetic islands. R. F. Wang, C. Nisoli, R. S. Freitas, J. Li, W. McConville, B. J. Cooley, M. S. Lund, N. Samarth, C. Leighton, V. H. Crespi, and P. Schiffer,, Nature 439, 303–306 (2006).

[2] Melting artificial spin ice, Vassilios Kapaklis, Unnar B. Arnalds, Adam Harman-Clarke, EvangelosTh. Papaioannou, Masoud Karimipour, Panagiotis Korelis, Andrea Taroni, Peter C. W. Holdsworth, Steven T. Bramwell, and Björgvin Hjörvarsson, New Journal of Physics 14 (2012) 035009 (10pp), IOP Select & highlight selection of 2012

[3] Thermalized ground state of artificial kagome spin ice building blocks, Unnar B. Arnalds, Alan Farhan, Rajesh V. Chopdekar, Vassilios Kapaklis, Ana Balan, Evangelos Th. Papaioannou, Martina Ahlberg, Frithjof Nolting, Laura J. Heyderman, and Björgvin Hjörvarsson, Applied Physics Letters 101 (11) , art. no. 112404

[4] Thermal fluctuations in artificial spin ice, Vassilios Kapaklis, Unnar B. Arnalds, Alan Farhan,Rajesh V. Chopdekar, Ana Balan, Andreas Scholl, Laura J. Heyderman and Björgvin Hjörvarsson, Nature Nano DOI: 10.1038/NNANO.2014.104

[5] The importance of the weak: Interaction modifiers in artificial spin ices, Erik Östman, Henry Stopfel, Ioan-Augustin Chioar, Unnar B. Arnalds, Aaron Stein, Vassilios Kapaklis, and Björgvin Hjörvarsson, Submitted.

[6] Thermal transitions in nano-patterned XY-magnets, Unnar B. Arnalds, Martina Ahlberg, Matthew S. Brewer, Vassilios Kapaklis, Evangelos Th. Papaioannou, Masoud Karimipour, Panagiotis Korelis, Aaron Stein, Sveinn Olafsson, Thomas P. A. Hase, and Björgvin Hjörvarsson, Appl. Phys. Lett. 105, 042409 (2014); http://dx.doi.org/10.1063/1.4891479

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Tuesday 10.10.17, 13:30-14:00

Applications of polarized neutron scattering to guide development of novel functional heterostructures

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Novel electric and magnetic properties can be achieved in materials engineered at nanometer dimensions. Examples include conducting or magnetic interfaces between materials that are neither conducting nor magnetic. New functionality stems from the atomic, charge, spin or orbital structure of the interface. With an understanding of interface structure, electric and magnetic degrees of freedom may be controlled, ideally at room temperature, to achieve synthetic magnetoelectric coupling in a nanocomposite or possibly to control spin textures in topological materials.

In this talk I describe applications of polarized neutron reflectometry (PNR) and small angle neutron scattering (SANS) with polarized neutron beams to probe magnetic interfaces in heterostructures and nanocomposites as functions of magnetic and electric fields. In one application, I discuss the origin of a novel form of magnetism in nominally antiferromagnetic $BiFeO_3$ (BFO) when sandwiched between $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) layers. Our results exclude charge transfer, intermixing, strain and octahedral rotations/tilts as dominating mechanisms for large uncompensated magnetization we see in thin BFO layers. We show that the BFO is simultaneously ferrimagnetic and ferroelectric to 200 K.

A second application illustrates the use of ionic liquids (IL) to reversibly switch the ferroelectric (FE) polarization of large area $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) films. Control of the polarization enabled us to show that hole accumulation and depletion induced by the FE polarization leads to a reduction or an enhancement, respectively, of the interface magnetism. IL-assisted FE gating may enable new applications of magnetoelectric coupled multiferroics—ones that operate at room temperature.

Work supported by the Office of Basic Energy Science, U.S. Department of Energy, Divisions of Materials Science and Scientific User Facilities, and ORNL Lab Directed Research and Development.

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Tuesday 10.10.17, 14:00-14:15

Neutron Zeeman beam-splitting for the investigations of magnetic nanostructures

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We have investigated magnetically non-collinear structure in a bilayer Fe-Gd film on a float glass substrate. The spatial neutron beam-splitting was observed in grazing incidence geometry at low magnetic fields applied parallel to the film surface. Using the Bitter technique, small magnetic clusters with a diameter of about 0.5 μm were observed in the film. The total area of the clusters surface consisted of about 5 % from the film surface. The magnetic induction value inside the magnetically non-collinear clusters was directly extracted by the Zeeman beam-splitting method. This magnetization curve corresponds to the hysteresis loop measured by macroscopic magnetometric methods MOKE and VSM for the entire film. The neutron spin-flip probability measurements show that the vector of magnetic induction in non-collinear clusters becomes collinear to the magnetic induction in the film for the applied field of about 400 mT. The beam-splitting can be applied as a direct sensitive micromagnetic method for the investigation of magnetically non-collinear nanostructures likes as patterned films, domains for perpendicular magnetic recording, etc. The results were published in [1]. The direct neutron methods for the investigations of magnetic films (Larmor precession, Zeeman beam-splitting and neutron spin resonance in matter) were described in our review [2]. For the robust interpretation of the experimental data we have used our program *SimulReflec* for the transformation of two-dimensional maps of intensity into different coordinate representations for off-specular scattering [3] and Zeeman beam-splitting [4].

We acknowledge JINR-Romania scientific project No. 219/10.04.2017, items 60 and 61.

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[3] F. Ott, S.V. Kozhevnikov, J. Appl. Crystal., **44**, 359 (2011).
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Tuesday 10.10.17, 14:15-14:30

Polarised Neutron Reflectometry Applied to *In-Situ* Thin Film Growth

Wolfgang KREUZPAINTNER[1], Sina MAYR[1], Jingfan YE[1], Birgit WIEDEMANN[1], Alexander BOOK[1], Amitesh PAUL[1], Thomas MAIROSER[2], Andreas. SCHMEHL[2], Alexander HERRNBERGER[2], Jochen STAHN[5], Jean-Francois MOULIN[4], Panagiotis KORELIS[5], Martin HAESE[4], Matthias POMM[4], Peter BÖNI[1], and Jochen MANNHART[3]

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Thin magnetic layers and heterostructures thereof are the basic building blocks of a large number of magneto-electronic devices. Their performance strongly relies on the magnetic properties of the layers they consist of. These are functions of the layers' morphology and microstructure and on the coupling between them. Since these parameters can change during the process of growth, it is important for the understanding and optimisation of magnetoelectronic devices to not only accurately monitor the structural but also the magnetic properties during the process of growth.

While the structural characterisation of thin films during growth by various techniques is common practice (as e.g. commonly done by RHEED/LEED, STM or synchrotron radiation), the *in-situ* measurement of the magnetic properties of films using (polarised) neutron reflectometry is a challenging task. Within a collaboration of TU München, University Augsburg and MPI Stuttgart, we operate a mobile sputtering facility for the growth and *in-situ* monitoring of magnetic multilayers, which can be installed at suitable neutron beamlines. In our contribution, the current state of the setup and recent experiments of polarised *in-situ* neutron reflectivity carried out at the AMOR beamline at PSI will be presented, where the Selene neutron optical concept allows very fast polarised neutron reflectivity measurements to be performed within as little as 15min per spin direction whilst keeping the sample aligned in the neutron beam at all times.

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Tuesday 10.10.17, 15:00-15:30

Neutron scattering techniques reveals the structure and dynamics lipid non-lamellar phases at the solid/liquid interface

Tommy NYLANDER[1,2], Olaf SOLTWEDEL[3, 4], Marina GANEVA[5], Christopher HIRST[1], James HOLDAWAY[1], Marianna YANEZ ARTETA[1], Maria WADSÄTER[1], Justas BARAUSKAS[6, 7], Henrich FRIELINGHAUS[5], Olof HOLDERER[5]

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Non-lamellar lipid based self-assembly structures have been increasingly recognized as important for living systems. Understanding the biological implication as well as the application of such interfaces, for e.g. drug delivery and other biomedical application, requires the development of well-defined model system [1]. We will discuss how to provide lipid based biofunctional surface films beyond supported bilayers, where the structural changes of deposited lipid can be controlled based on measurements using neutron techniques. This will be achieved by forming non-lamellar lipid liquid crystalline surface layers by means of spin-coating the constituting lipids followed by hydration of the lipid layer will be demonstrated [2]. The structure and dynamics in these nano-structures films formed by mixtures of soy phosphatidylcholine (s-PC) and glycerol dioleate (GDO) at the silicon-aqueous interface were studied by grazing incidence neutron spin echo spectroscopy (GINSES), specular and off-specular neutron reflectometry and small angle x-ray diffraction (SAXD) [3]. Neutron reflectometry measurements and SAXD showed that reverse hexagonal (H_{II}) and micellar cubic phase (Fd3m) layers at the solid/liquid interface can be formed by changing the lipid composition. For the cylindrical hexagonal phase only, orientation of the liquid crystalline phase was identified. The size of the liquid crystalline domains was 1μm as estimated from the width of the diffraction peaks. GINSES revealed that both phases form rather rigid films. In comparison the H_{II} film was more flexible, appearing as a modified undulation spectrum of the cylinders due to the interaction with the substrate. The results will be discussed in terms of potential neutron techniques to reveal these intriguing systems.

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Tuesday 10.10.17, 15:30-16:00

Molecular membrane biophysics

Maikel RHEINSTADTER[1]

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Our lab is running a research program in membrane biophysics. We use X-ray and neutron beams to study molecular structure and dynamics in membranes in-situ, under physiological conditions [1]. We study nanoscale diffusion within and across membranes, the effects of small molecules on membrane properties, the interaction with common drugs, such as aspirin, ibuprofen and cortisone, and their side effects. We detect and characterize membrane rafts and peptide interactions in Alzheimer's disease. Experiments are complemented by molecular dynamics computer simulations. I will talk about current topics in membrane biophysics, nano- and personalized medicine, the associated experimental challenges and present exciting recent results and biomedical applications.

[1] http://www.rheinstaedter.de/maikel/publications/publications.htm

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Tuesday 10.10.17, 16:00-16:15

Elucidating lipid membrane spreading on surfaces by time-resolved neutron reflectivity

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The formation of supported lipid bilayers (SLB) on hydrophilic substrates through the method of unilamelar vesicle fusion is used routinely in a wide range of biophysical studies. In an effort to control and better understand the fusion process on the substrate, many experimental studies employing different techniques such as quartz crystal microbalance (QCM), surface plasmon resonance (SPR) and in-situ atomic force microscopy (AFM), have been devoted to the elucidation of the fusion mechanism. The general picture drawn from different studies concerning the steps involved in the formation of SLB via vesicle fusion includes an initial adsorption of intact vesicles on the substrate, subsequent rupture and finally their spreading leading to coalescence and full coverage.

Neutron and X-ray reflectivity offer the possibility to obtain a detailed nanometer scale picture of the molecular distribution at the solid liquid interface and have been implemented in the past for the study of vesicle fusion. In the present work we revisit the use of neutron reflectivity under a constant solution flow setup and low vesicle concentrations in order to capture the reflectivity of the system during the various stages of the SLB formation process. Model fitting of the reflectivity curves acquired during the fusion of phospholipid vesicles on silicon oxide provide interesting insights in relation to results from real-space techniques. In particular our observations compare favorably with recently proposed mechanism (Biophys. J. **2009**, 98, 85) that considers membrane patch edges as high affinity surfaces for vesicle adsorption.

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Tuesday 10.10.17, 16:15-16:30

Depth resolved GISANS from liquid solid interfaces

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The development of thin layers and nano-devices inspire future technologies. In this context GISANS (Gracing incidence small angle neutron scattering) experiments became an invaluable tool for the investigation of ordering at an interface. However, for the study of solid-liquid boundaries the method is challenging, since typically, due to the low absorption of neutrons, the surface signal has to be separated from bulk scattering. When using time of flight methods for one setting of the incident angle a wide range of penetration depth can be covered. By using this approach the near surface structure of polymer micelles can be extracted with a certain degree of depth sensitivity [1].

To quantitatively analyse the intensities of such depth resolved data sets we present a novel data treatment approach. By calculating the penetrating flux at each depth from a convolution of the penetration depth and the two dimensional resolution function, it is possible to quantify the depth dependent contribution to the scattering signal. The contribution of each angle of incident as well as the impinging wavelength is evaluated for each individual setting of the instrument including the beam divergence and monochromaticity regarding the penetration depth.

For certain conditions and a sufficient number of scattering data sets it is possible to use a reverse linear transformation to deconvolute the effect of the resolution and reconstruct the structure of the ordering in the vicinity of the interface with depth sensitivity.

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Wednesday 11.10.17, 09:00-09:30

Using GISANS and Reflection to Understand the Structure of Colloidal Dispersions near Interfaces

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The structure of colloidal dispersions near solid interfaces is important as they are important in determining the rheology of fluids, properties of coatings, preparation of optoelectronic materials and the behavior of sensors. Neutron reflection measurements can determine the density and composition profiles perpendicular to the interface in the direction Q_z. Off-specular scattering and grazing incidence small-angle scattering provides (GISANS) information about the lateral structure in the plane of the interface (Q_x, Q_y). As the grazing angle of incidence of the incoming beam increases, it penetrates further and probes different average depths within samples. Calculation of the penetration depth is essential for quantitative models of scattered intensity and depends on sample properties such as the total scattering cross-section, the absorption and on instrument parameters such as the wavelength spread and beam divergence.

The calculations are tested with GISANS data measured for the self-organized structures formed by charge-stabilized colloidal particles with different sizes that were measured on two different instruments. [1] The results demonstrate that oriented single domain colloidal crystals can extend many micrometres towards the bulk from a solid interface. The results of GISANS measurements will be contrasted with the slit-smeared off-specular scattering measured with a conventional reflectometer. [2] Strong scattering from ordered interfacial structures that is modulated in the Q_x direction can, when smeared, significantly perturb data that could mistakenly be interpreted simply as components of the specular signal.

The combination of different measurements is important for the successful interpretation of results and to determine the three-dimensional structure that exists at solid/liquid interfaces.

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Wednesday 11.10.17, 09:30-10:00

Polarised neutron Reflectivity and the Magic Angle Tuning of the Contrast

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We report a possible new experimental technique which enables a spectrum of a polarised neutron reflectivity profile to be obtained for a reference magnetic layer. This technique allows for a more precise structural determination at interfaces, than the existing spin up and spin down approach. This new experimental approach provides a means of varying the scattering length density (contrast) of the reference layer without the need of deutration. It relies on the ability to magnetise the reference Fe layer permanently. These steps will enable a fine tuning capability of the scattering length density (Nb) of a reference layer by simple rotation of the sample with respect to the incident polarised beam. Hence the measured reflectivity profiles can provide a tuneable sensitivity to highlight specific structural features of a complex system adsorbed at the substrate bulk interface without requiring any changes to the actual system under investigation. This approach, in combination with the conventional isotopic exchange measurements, will provide comprehensive structural details not currently available, in particular for multifaceted biological systems.

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Wednesday 11.10.17, 10:00-10:15

Operando neutron reflectometry study of lithium enriched deposition on metal electrode in contact with liquid electrolyte

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The performance characteristics of modern electrochemical energy storage devices are largely determined by the processes occurring at charge separation interfaces and causing modifications of the interface structure. Thus, lithium ion batteries with liquid electrolytes are characterized by the appearance of a specific formation on the electrode surface known as solid-electrolyte interphase (SEI). The structural properties of this layer (thickness ~10 nm) are also important in respect with possible lithium "moss" growth at the electrode-electrolyte interfaces upon battery cycling, the phenomenon which is a problem from the viewpoint of safety. In this regard, in deep structural characterization of the discussed formations at nanoscale in operating devices is of current interest for the regulation of subsidiary effects in using electrochemical interfaces with lithium containing electrolytes. The corresponding operando studies of nanoscale are a complicated problem which requires elaborate designs of experiment and applications of various methods to monitor the interfaces of interest [1]. Among such methods, neutron reflectometry (NR) is one of few techniques which provide a sensitivity to berried or hidden interfaces due to high penetration power of thermal neutrons.

In the given presentation, the NR possibilities for studying the formation of SEI and its influence on the Li plating on a thin (thickness 50 nm) copper electrode depending on the composition of the electrolyte is considered. For this purpose, the NR experiments are carried out (GRAINS horizontal reflectometer, IBR-2 reactor) for the interface with a standard electrolyte mixture (lithium perchlorate in propylene carbonate) and with the same electrolyte but where a non-electroactive component (tetrabutylammonium perchlorate) is added. The additives of such kind are now tested as potential suppressers of parasitic formations at the interfaces in lithium ion batteries. The nanoscale modifications of the lithium enriched layer formed on the electrode in different conditions are analyzed basing on the data of specular reflectivity of thermal neutrons obtained in the operando mode.

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Wednesday 11.10.17, 10:45-11:15

Magnetic SANS as a probe to disclose internal interfaces

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Small-angle neutron scattering (SANS) is a very powerful technique for the investigation of magnetic materials, since it provides information from within the *bulk* of magnetic media and on a length scale between a few nanometers and a few hundred of nanometers (~ 1-300 nm). In this talk, we summarize recent theoretical and experimental work in the field of magnetic SANS of bulk ferromagnets [1]. The response of the magnetization to spatially inhomogeneous magnetic anisotropy and magnetostatic stray fields is computed using micromagnetic theory, and the ensuing spin-misalignment SANS is deduced. This approach goes beyond the traditional description of SANS in terms of particle form and structure factors. Analysis of experimental magnetic-field-dependent SANS data corroborates the usefulness of the approach, which provides important quantitative information on the magnetic-interaction parameters such as the exchange-stiffness constant, the Dzyaloshinski-Moriya interaction, the mean magnetic anisotropy field, or the mean magnetostatic field due to jumps ΔM of the magnetization at internal interfaces. Besides the value of the applied magnetic field, it turns out to be the ratio of the magnetic anisotropy field H_p to ΔM, which determines the properties of the magnetic SANS cross section of bulk ferromagnets; specifically, the angular anisotropy on a two-dimensional detector, the asymptotic power-law exponent, and the characteristic decay length of spin-misalignment correlations. Unpolarized and polarized neutron data on selected magnetic materials (e.g., Nd-Fe-B magnets, Fe-based soft magnets, nanocrystalline Gd) will be discussed. We put special emphasis on the discussion of the disordering effect of internal interfaces (grain boundaries) on the magnetization process and on their signature in the magnetic SANS cross section.

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Wednesday 11.10.17, 11:15-11:30

Magnetic structure of ferrite nanoparticles on a square lattice

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Long-range ordered arrangements of magnetic nanoparticles are fundamentally interesting for the investigation of dipolar coupling [1, 2]. For single domain magnetic nanoparticles arranged in a dense square lattice, electron holography experiments and numerical simulations show that dipolar interaction leads to a local super antiferromagnetic coupling [3, 4, 5].

In order to investigate the long-range interparticle coupling, we prepared square arrangements of ferrite nanocubes. The lateral structure and magnetic order are studied using grazing incidence small-angle x-ray and neutron scattering, respectively. The results are compared to simulations of ordered spin ensembles obtained by a combination of the BornAgain software [6] with Monte Carlo simulations.

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Wednesday 11.10.17, 11:30-11:45

Magnetic nanomaterials

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Magnetic nanomaterials and their assembly in highly correlated structures are of great interest for future applications as e.g. spin-based data storage media or as material for magnon-spintronics. These systems exhibit unique physical properties like superparamagnetism or symmetry breaking emerging due to their limited size. Individual nanomaterials can be combined as building blocks for so called superstructures where the combination of the different functionalities creates a novel multi-functional system.

Recently, more and more well-defined nanoobjects became available and the advances in measurement methods allow a characterization of these systems. For example, single micrometer-sized three-dimensional magnetic nanoparticle assemblies are available, exhibiting a high degree of structural order close to that of an atomic crystal [1,2]. These systems provide a good basis for the magnetic investigation of nanoparticle superstructures.

The work to be presented focuses on the fundamental structural and magnetic research on such objects and their functionalization. For the investigation we make use of different complementary measurement methods like small angle x-ray and neutron scattering or using microresonators, which provide the necessary sensitivity for the investigation of magnetic properties of a single nano- or micrometer-sized object using ferromagnetic resonance (FMR) [3].

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Wednesday 11.10.17, 11:45-12:00

The spin structure of highly ordered arrangement of magnetic nanoparticles

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Highly ordered arrangements of magnetic nanoparticles are fundamentally interesting regarding the understanding of magnetic interactions and for a rational design towards potential applications in information technology and spintronics.
Long range ordering between magnetic nanoparticles in two and three-dimensions is obtained by assisted self-assembly using pre-patterned substrates with feature size of the same order of magnitude as the diameter of the nanoparticles.
In this contribution, we will report on the first steps of this program, that are the structural characterization of patterned silicon substrates by Grazing Incidence Small Angle X-ray Scattering (GISAXS) on the laboratory high brilliance GALAXI instrument [1] with data analysis using the BornAgain software [2] also the structural and magnetic characterizations of monolayers of $CoFe_2O_4$ nanoparticles and directed self-assembly of silica nanoparticles into patterned silicon substrate.

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[2] http://www.bornagainproject.org

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Wednesday 11.10.17, 13:00-13:30

Advances in Neutron Reflectometry Techniques: Coherent Summing and Refractive encoding.

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Reflectometry is a powerful technique used to determine the density, separation, composition and quality of interfaces. Compared to electromagnetic radiation it does however suffer from the limits of the relatively feeble brilliance of neutron sources. Higher intensity from a more open collimation is traditionally thought to be paid for in looser resolution. Given that angular information of the neutron path is preserved in specular reflectivity one can use the detector resolution to reduce the uncertainty in reflection angles and hence improve the resolution. The result is, for flat samples, a very large divergence can be exploited with no significant loss of resolution. There is an added benefit with bent samples where the spread of the reflected beam does not entail a loss of resolution either. We call the data reduction algorithm coherent summing [1]. In addition to this software development we have also been commissioning the technique of refractive encoding [2,3] whereby a white beam is reflected from a flat sample and subsequently refracted by a prism surface, exploiting the dispersion to measure the wavelength. The gain of this method is potentially enormous and initial tests have shown we can measure reflectivity less than 10^{-6}. Both methods show promise of new science with small samples or shorter kinetic time resolution.

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Wednesday 11.10.17, 13:30-13:45

Opportunites in Surface Scattering at the European Spallation Source

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The European Spallation Source, which is under construction in Lund, Sweden, will provide new opportunities for the development of surface sensitive scattering techniques using neutrons.

The suite of 15 instruments now under construction includes a number of instruments that will provide capabilities for surface sensitive measurements of structure and dynamics.

Here we will give an overview of those instruments currently under construction and discuss the opportunities for future instruments that could make optimum use of the ESS source design to advance the state of the art in these types of measurement.

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Wednesday 11.10.17, 13:45-14:00

The neutron spin echo spectrometer J-NSE: the past and the future

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The J-NSE neutron spin echo spectrometer at MLZ provides access to a rather unique range of length- and time-scales relevant in soft matter systems. Neutron spin echo spectroscopy has been used to study thermal fluctuations and diffusion in soft matter systems, for example domain motion of proteins [1,2], diffusion in crowded environment [3] or membrane fluctuations [4] at interfaces under grazing incidence conditions. under natural (physiologically relevant) conditions. We present scientific highlights and instrumental developments at the J-NSE in the last years, as well as a look into the future of the J-NSE after the ongoing major instrumental upgrade for a significant increase in resolution [5] by exchanging the main solenoids by superconducting coils providing an optimized field shape.

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Wednesday 11.10.17, 14:00-14:15

Reflectometers at the European Spallation Source

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The European Spallation Source (ESS) is the next generation neutron source being build in Lund, Sweden. With its long pulse time structure, small angle and reflectometry instruments can profit the most from the large beam brilliance the source will provide. Recently, the preliminary design phase for the first instruments was concluded and the initial installation scope has been defined together with an early upgrade path.

We will present the two initial reflectometers, ESTIA and FREIA, which will be installed at ESS and their expected day one performance at 2 MW proton beam power. Due to their different concepts and optimization strategies, these instruments will cover the full range of the reflectometry science case while each will have unique possibilities for novel experiments, including focusing on tiny samples and a few seconds time resolved measurements. A short overview of the available sample environment and possible upgrades will conclude the presentation.

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Wednesday 11.10.17, 14:15-14:30

Instrumental developments for grazing incidence neutron scattering experiments for nano-scale tribology studies

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Neutron waveguides can be used to enhance intensities near (or inside) the waveguide for surface characterizing grazing incidence scattering experiments. This tool we applied for characterizing lipid membrane dynamics that have not been accessible in a grazing incidence neutron spin-echo spectroscopy (GINSES) experiment before [1]. We observed a clear signature for a viscoelastic response of the lamellar bilayer stack confined by the solid surface. The elastic surface wave modes at relatively large wavelengths agreed with a theory from Romanov et al.

The GINSES measurements have been performed at the SNS-NSE spectrometer in Oak Ridge where a relatively large wavelength band (5 to 8Å) was used. For staying safely below the critical angle of total reflection, we used a neutron prism that corrected the scattering depth of the evanescent wave to take a rather constant value. In this way, the measurement could be allocated to a well-defined depth.

These tools would allow for a broad range of near surface structure and dynamics studies that can be connected to tribological effects. In this way, we hope to open new perspectives for a relatively young field of science.

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Wednesday 11.10.17, 15:00-15:15

Aside from neutron instruments: thin film fabrication by molecular beam epitaxy at the Jülich Centre for Neutron Science

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Rational design and implementation of new generations of functional materials for energy conversion and storage, requires better fundamental understanding of these systems along with the ability to predict their properties accurately. [1, 2, 3] Utilizing thin film systems, the knowledge of the driving parameters to obtain them in high quality is crucial [4]. Molecular Beam Epitaxy (MBE) proves to be a versatile method to grow high quality and high purity epitaxial films with low intrinsic defect concentrations and atomic-layer control.

At the JCNS thin film laboratory, we run an oxide MBE system for the growth of various types of samples, i.e. "classical" magnetic thin films, transition metal oxide heterostructures or just thin gold films for soft matter studies, acting as defined surfaces. However, every sample system comes with its own challenges which makes thin film growth a research topic on its own.

In the presentation, we will give an overview for high quality metal and complex oxide thin film systems all fabricated in the JCNS thin film laboratory, like $SrCoO_x$, $La_{1-x}Sr_xMnO_3$, Fe_4N or Cu/Fe multilayers. The focus lies on stoichiometry, morphology and thickness precision and detailed information about the possibilities in sample fabrication for users will be given.

For quasi in-situ neutron reflectometry on thin films which are sensitive to ambient air a small versatile transfer chamber can be utilized for sample transfer and measurement from the MBE laboratory to the neutron instrument MARIA [5]. Both, the MBE setup and the transfer chamber may be booked in combination with an application for beam time at neutron instruments like MARIA.

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Wednesday 11.10.17, 15:15-15:30

Probing magnetic dynamics at interfaces using waveguide PNR

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In this work we propose a method for detection of neutron inelastic scattering on magnetic excitations in thin films and interfaces. Method is based on using of resonator (waveguide) structures [1,2] and peculiarities of inelastic scattering of polarized neutrons on magnetic excitations [3]. Method requires no separation on neutron energy, similar to Ref [4], and allows detecting magnetic excitations with ultra-small Q (down to 0.01 $Å^{-1}$).

We present several experimental examples made at angle-dispersive reflectometer NREX on different magnetic systems with magnetic layers varying from classical 3d ferromagnets to exotic half-metallic oxides.

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Wednesday 11.10.17, 15:30-15:45

Octagonal neutron guide for the horizontal sample reflectometers

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Horizontal sample reflectometers, having vertical scattering plane, can gain intensity through horizontal beam focusing. It means that such type of instruments favours “wide” beam while reactors usually provide “tall” beams. Neutron guides are usually produced of rectangular shape due to technical reasons. Important consequence is that the problem of the neutron transport can be divided in two independent, e.g. regarding vertical and horizontal planes separately.

We have investigated the possibility of octagonal guide as a way to transport neutrons to the vertical scattering plane reflectometer. If to introduce some inclined plane it would be possible to “pump” neutron beam phase space density from one plane to another. By means of the octagonal guide section which adiabatically changes its shape it would be possible to transform guide form “tall” to “wide” gaining high horizontal divergence for further focusing at the sample position.

We have investigated the optical properties of such octagonal guide: what length is needed to fully transform the beam, how does it depend on the wavelength, initial cross-section and divergence, what is the effectiveness of such transform. Also the results will be shown for the particular case of the horizontal sample reflectometer LIRA which is proposed for the high-flux PIK reactor, Gatchina, Russia.

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Wednesday 11.10.17, 15:45-16:00

Neutron Depth Profiling at a focused neutron beam to study Li-ion transport in thin-film batteries

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In operando observations of Li transport in all-solid-state thin-film batteries during fast (dis)charge cycling, as well as the study of mechanisms of battery aging become possible at a new Neutron Depth Profiling (NDP) setup of JCNS, using the focused neutron beam of reflectometer MARIA (MLZ). This arrangement allows for sufficiently high counting rates necessary for fast, about tens of seconds, measurements under the requirement of a fine, of an order of 10 nm, depth resolution.

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Wednesday 11.10.17, 16:00-16:15

WASP Wide Angle SPin echo instrument for spectroscopy not just on surfaces

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All functioning neutron spin echo spectrometers essentially use the IN11A design where the precession field is generated by a long solenoid along the neutron beam. This construction limits the angular coverage of the instruments. Last century there have been two tries to make a wide angle coverage neutron spin echo instrument. IN11C uses a flattened solenoid and has been in use since then, having a 30 degree-wide angular coverage but a very limited resolution. This instrument was practically trading intensity for resolution. The SPAN instrument at HZB used pair of coils in the anti Helmholtz configuration creating an azimuthally symmetric magnetic field; which in theory could allow a nearly 360 degree detector coverage. WASP will use an improved SPAN construction and it aims to have a 1000 times higher detected intensity than IN11A while the resolution remains the same.

After a decade of planning[1-3], with the financial contribution of Jülich WASP has finally taken off, the neutron guides have been installed, the main coils are installed, tested and undergoing magnetic field commissioning. Neutron commissioning should start in fall 2017. This new spin echo instrument is aimed at extending previous studies on IN11C, which includes among many subjects diffusion and adsorption dynamics on carbon surfaces [4-5].

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Thursday 12.10.17, 09:00-09:30

Neutron Scattering for Studying Structure and Dynamics of Stimuli Sensitive Polymer Coatings

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For fabrication of stimuli responsive coatings one challenge is to generate stable films which are still mobile and sensitive to outer parameters. The talk will focus on 2 different types of thin polymer films at solid interfaces: 1) films formed by deposition of hydrogel microgels and 2) polymer brushes. Both architectures have in common that they consist of N-isopropylacrylamide (NIPAM) monomers.
During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest and were studied by several techniques like microscopy and light scattering. These polymer particles show thermoresponsive behaviour and can therefore be classified as “smart” materials. By copolymerisation with organic acids such as acrylic acid (AAc) the temperature of the volume phase transition as well as the swelling ratio can be influenced. Moreover charged copolymers are sensitive to changes in pH and ionic strength. Our work focuses on the fabrication of stimuli responsive films and on the effect of geometrical confinement on the phase volume transition of these microgel particles [1]. The effect of cross-linker and co-monomers on the swelling behaviour and on the elasticity is presented [2]. The second example is coating with PNIPAM brushes synthesized via ATRP and *grafting from* method [3].
Beside pH, temperature light is a very efficient stimulus, since it can trigger quite fast and local the volume phase transition. Therefore additives like surfactants with azobenzene groups [4] and gold nanoparticles [5] are embedded within both microgels and brushes. In case of gold nanoparticles, the change in optical properties of microgels and brushes and the impact of gold nanoparticles as hot spots is studied.
For a better understanding of the structure-function relation it is essential to get insight into the distribution of the gold nanoparticles within the polymer coatings. Therefore neutron and x-ray reflectometry are suitable methods [3,7]. Adsorption at the interface affects the volume phase transition due to the compression of the gel structure. In this context we studied the structure and the dynamics of the gels in bulk and at the interface with SANS and NSE in bulk and under grazing incidence (GISANS, GINSE) [6,7].

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Thursday 12.10.17, 09:30-10:00

"Near surface dynamics of adsorbed and tethered polymer systems: Results and instrumental aspects"

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The physical properties of stimuli-responsive microgels and polymer brushes still attract great interest in basic research. This research leads to a lively discussion of potential technical applications. Prominent examples are systems, which undergo a temperature induced phase transition as the sample temperature changes.

Microgel particles can be organized as ultra-thin films at solid surfaces, which leads to changes in the swelling behavior and shifts the LCST with respect to the bulk phase. These findings raise the question how the interactions with the solid surface affect the inner structure and dynamics of the adsorbed microgel particles. [1,2]

Polymer brushes as polymers tethered at one end to a solid surface are another prominent example of such architectures. Among them, thermoresponsive polymer brushes made of P(MEO2MA-co-OEGMA) are promising biocompatible candidates for smart coatings designed for biotechnological applications.

Here, we focus on neutron spin echo spectroscopy experiments in transmission and reflection geometry on both types of systems. [3]

Beside the scientific results of the scattering experiments we discuss instrumental aspects, providing a further improvement of the method and adaption to the requirements of experiments on thin layers of colloids and polymer systems at solid substrates

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Thursday 12.10.17, 10:00-10:15

Description of poly(ethylenepropylene) confined in nanopores by a modified Rouse model

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A recent model for unentangled polymer chains in confinement [1] is scrutinized by small-angle neutron scattering (SANS) with respect to its static prediction, the single-chain structure factor. We find a remarkable agreement although the model simplifies the effect of the confinement to a harmonic potential. The effective confinement size from fits of SANS data with the model agrees well with the actual pore size. Starting from this result we discuss the possibility of an experiment on the dynamic structure factor predicted by the model. It turns out that such an experiment would need a large ratio polymer dimension/pore size which is difficult but not impossible to achieve. [2]

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Thursday 12.10.17, 10:45-11:00

In-situ time of flight neutron reflectometry study of the swelling and exchange kinetics of multi-stimuli responsive PNIPAM based block copolymers

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Thermoresponsive polymers can react with a strong change in volume towards small changes in temperature which makes them attractive for a manifold selection of applications. [1] While the underlying mechanisms of such polymers in solution are well understood, less is known about thermoresponsive polymers in thin film morphology. However, this is surprising since these polymer thin films have great potential in application areas such as sensors, biomedical applications and smart surface coatings. [2, 3] In this context, the most studied polymer is poly(N-isopropylacrylamide) (PNIPAM) which exhibits a lower critical solution temperature (LCST) at 32°C and therefore is especially applicable in the biomedical field. [4]

In order to increase the pool of studied thermoresponsive polymers and to gain a better fundamental understanding of thermoresponsive thin films we focus on the analysis of the swelling and exchange behavior of newly synthesized block copolymers. These copolymers comprise a PNIPAM block and a poly(sulfobetaine) (PSB) block. Via in-situ time of flight neutron reflectometry (TOF-NR) we detected the swelling kinetics of PSB-b-PNIPAM films in saturated D_2O atmosphere. Furthermore, we followed in-situ the exchange kinetics when replacing the D_2O with an H_2O atmosphere. With this sophisticated technique a reasonable Q_z range is accessible and the kinetic processes can be followed with a high time resolution. A theoretical model is applied to describe the swelling and exchange and detailed insights about the mechanisms of D_2O diffusion inside the film and the D_2O to H_2O exchange are obtained. Fourier transform infrared spectroscopy and white light interferometry measurements are performed as well, to complete the collected data and to confirm the applied theoretical model.

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Thursday 12.10.17, 11:00-11:15

Inner structure and dynamics of the stimuli-responsive polymer microgel particles adsorbed on surface

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First results of the simultaneous application of surface sensitive scattering techniques (e.g. grazing incident small-angle neutron scattering (GISANS) and neutron spin echo spectroscopy (GINSES), neutrons reflectivity (NR)) and a numerical simulations of the experiment in the framework of the Distorted Wave Born Approximation (BornAgain software package [1]) are presented.

Scattering experiments on soft matter systems such as adsorbed microgels or polymer brushes often give only partial information about the inner structure of the polymer system. In this contribution, we discuss how the detailed inner structure of adsorbed microgel particles can be reconstructed by a combination of the obtained data [2] and simulation of the GISANS scattering pattern.

We used stimuli-responsive microgel (p-MeO2MA-co-OEGMA) and (PNIPAM-BIS) particles [3, 4] with different comonomer or cross-linker contents absorbed on a Si substrate.

Stimuli-responsive microgel particles open wide opportunities of applications as coatings on implants with possibility of drug release. That in turn demands a clear understanding of polymer surface properties with respect to a different stimulant (temperature, pH), which allows to tune them in a controlled way.

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Thursday 12.10.17, 11:15-11:30

Nanorheology: Using neutrons to discover the dynamics of biological membranes

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Here we present Grazing Incidence Neutron Spin-Echo Spectroscopy (GINSES) data to measure dynamic membrane properties close to a solid interface. As an example we show results of membrane dynamics of a phospholipid (L-α-phsophatidylcholin, SoyPC) membrane multilayer stack on a solid substrate (silicon). From this sample we directly measure local interaction and friction parame- ters. This is achieved by Grazing Incidence Neutron Spin Echo Spectroscopy (GINSES), where an evanescent neutron wave probes the fluctuations in the sample close to a rigid interface. With this method it is possible to access length scales in the nano- to micrometer region and energies on the order of μeV . Only by using a new neutron resonator structure we achieved the required intensity gain for this experiment. During our investigations we found an additional excitation mode of the phospholipid membrane that has not been reported before and only became visible using the new methodology. We assume this mode is playing a role in the self-stabilization mechanism of phospholipid membranes. Knowledge about this mechanism can also be applied in the study of other biological membranes. Thus, this new methodology has the capability to probe the viscoelastic effects contributing to lubrication and thus become a new tool for tribology on the nanoscale and has shown an hitherto unknown property of phospholipid membranes.

We correlate the results of the investigations of the dynamic properties of the phospholipid membranes with static measurements of the structure of those membranes, such as Grazing Incidence Small-Angle Neutron Scattering (GISANS) and Neutron Reflectometry. This correlation is both vital for a complete understanding of the interplay between dynamics and structure, as well as allows different avenues of approaches, where dynamical properties of the membrane are investigated on shorter length scales as well as longer times.

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Thursday 12.10.17, 11:30-12:00

Probing thin film nanostructures generated by block copolymer self-assembly using advanced scattering techniques

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Block copolymer self-assembly is a fascinating approach to fabricate functional nanostructured materials. Highly ordered nanostructures are achieved by micro-phase separation of the block copolymer. Incorporation of these nanostructures in devices typically requires a thin film geometry, which gives rise to morphological changes induced by the interface interactions. As a consequence, complex inner film morphologies can result, which may significantly deviate from equilibrium bulk morphologies. To fully characterize these nanostructures is an inherent challenge. With advanced scattering techniques the nanostructures of block copolymer films are probed in a non-destructive manner and with high statistical relevance [1]. In addition to surface structures commonly probed with imaging techniques, inner film structures are accessible, which is of high relevance for many applications such as in energy conversion and storage. Grazing incidence small angle neutron scattering (GISANS) can probe interface induced morphology transitions [2,3].

In-situ measurements give further insights into the morphology development during film preparation as well as in morphology transformations induced by changes of external control parameters. For example patterned diblock co-polymer thin films can be used as templates for an advanced anisotropic metal nanostructure fabrication [4,5].

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Thursday 12.10.17, 13:00-13:15

Instrument operations for the CANDOR reflectometer: handling and reducing data, modes of operation and current construction status

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The CANDOR white-beam reflectometer is under construction at the NIST Center for Neutron research. We will discuss the plans for handling and reducing the data from the instrument, which will be implemented in the web-based system currently in use on the 3 other reflectometry instruments at NCNR. The data will be stored in files with a NeXuS-compliant structure, but not in an HDF container.

The instrument has several planned modes of operation which will be discussed, including configurations with a convergent (not slit-defined) multiple-wavelength incident beam, a multiple-slit defined multiple-wavelength incident beam, or a single incident beam with either multiple wavelengths (0.4 to 0.6 nm) or a monochromatic 0.5 nm wavelength. The expected experiment types for each mode of operation will be discussed. For each of these incident-beam configurations, the detector array will be the same (multiple arrays of wavelength-selecting analyzer crystals with paired scintillation detectors arranged in a fan array to capture multiple scattered angles and scattered wavelengths simultaneously). The detector technology for the instrument is nearly complete, and a brief discussion of the detector system will also be presented.

The scientific program will be discussed, identifying experiment types that can most benefit from the efficiencies gained in the new instrument, as compared to a non-multiplexed reflectometer such as the existing ones at the NCNR.

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Thursday 12.10.17, 13:15-13:30

BornAgain: simulation and fitting framework for nuclear and magnetic GISANS

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A common software for the simulation and data analysis in the field of surface neutron and X-ray scattering is of key importance for scientists running their experiments at various neutron and synchrotron facilities. BornAgain [1] is a free and open-source project that provides scientists with the means to simulate and fit their specular, off-specular and GISAS data within a single framework. The name of the software, BornAgain, indicates the central role of the distorted-wave Born approximation in the physical description of the scattering process. The software is capable of modeling multilayer samples with smooth or rough interfaces, various types of embedded nanoparticles and various models to treat finite size effects and the coupling between the type and position of a particle. It also supports both nuclear and magnetic neutron scattering, offering the user a way to analyze polarized GISANS. Carefully designed for a broad community of users, BornAgain offers a modern graphical user interface with the possibility to perform real-time simulations and to fit experimental data. An advanced Python API lets experienced users create complex models. BornAgain is a multi-platform software released under the GPL3 license. It is adherent to object-oriented design, fosters a professional approach to software development and lays a solid foundation for future extensions in response to specific user needs.

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Magnetic field-shape optimization and new superconducting coils for the high-resolution neutron spin-echo spectrometer (J-NSE) at MLZ.

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Keywords: optimization, neutron, instrumentation, dynamics

An optimized shape of the magnetic field can reduce the intrinsic inhomogeneity inside cylindrical solenoids [1]. We present a semi-analytical method that has been developed to optimize the magnetic fields and to design new cylindrical magnetic coils with minimal intrinsic field-integral inhomogeneity for high-resolution NSE spectrometers [2]. Following this approach a set of new solenoids has been designed for the upgrade of the neutron spin-echo spectrometer (J-NSE) at MLZ. The new coils are fully compensated, superconducting solenoids that will enhance the resolution of the spectrometer by reaching higher Fourier times. Due to the lower intrinsic field inhomogeneity in the beam area the amount of required correction is expected to be reduced by over a factor 2.

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Thursday 12.10.17, 13:45-14:00

Connecting MARIA with the MBE system: Polarized Neutron Reflectivity of thin Co films in UHV conditions using portable transport chamber

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MARIA is a dedicated instrument for neutron reflectometry of thin films. However, due to limited space a UHV system for thin film growth and in-situ measurements cannot be placed on-site. Hence, up to now ultra thin films which are sensitive to ambient air have been fabricated in the MBE system located in the thin film laboratory nearby and were covered by protecting cap layers in-situ. However these layers may change the physical properties of the sample.

Recently, we have solved this problem by developing a handy mini UHV transport chamber which is capable for both, sample transfer and polarized neutron reflectivity (PNR) measurements in UHV [1]. In this work, we present PNR of Co thin films with varying thickness deposited on Pt buffered MgO(001) substrates. The samples were prepared in the MBE and measured at MARIA under UHV condition using transport chamber. During the measurement a field of 100 mT was applied parallel to sample surface. We found that the Co thin film is magnetically dead below 5 nm. However, magnetic moment in Co thin films evolves with increasing thickness and approaches to the bulk value (~1.7 μ_B) above 3 nm. In addition, we also measured PNR of Co thin films after exposing to the ambient air. The fitting of the PNR data shows that surface of the Co film get oxidised in air but is protected from contamination in UHV.

This project is part of the nanoscience foundry and fine analysis project (NFFA, www.nffa.eu) and has received funding from the EU's H2020 research and innovation programme under grant agreement N. 654360.

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Thursday 12.10.17, 14:00-14:15

Development of a foam cell for SANS measurements in the framework of a modular sample environment system

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Changing the sample or sample environment at neutron instruments within a reasonable amount of time, is important to reduce the downtime between individual experiments and user changes. This is especially critical for future high-flux neutron sources like the European Spallation Source (ESS). A strategy to enable quick sample environment changes is to design different sample environments fitting to a uniform base module or frame to allow a “plug&play”-type operation. In addition, standardization of the used hard- and software whenever possible is a great advantage. Together with our collaboration partners from the TU Munich and the University of Bielefeld we develop such a modular sample environment for different neutron experiments with soft matter samples. Here, we report on the contribution of our group to this project, namely the development and construction of a sample environment for small angle neutron scattering (SANS) at macroscopic liquid foams. The few publications dealing with SANS at aqueous foams all use a very similar sample cell, first introduced by Axelos and coworkers [1]. This cell is based on an acrylic glass cylinder with quartz windows for the neutron beam and foam formation is realized by bubbling gas through a porous glass or metal plate. Our foam cell also follows this approach, but we will extend the range of possible experiments by adding a temperature control unit, a camera for optical surveillance of the foams and a movable sample stage, which allows automated sample changing.

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Thursday 12.10.17, 14:15-14:30

Fitting Reflectometry Data Revisited

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Fitting reflectometry data is often a tedious task which requires a lot of fine tuning by an experienced user. Methods such as bayesian analysis can help reducing this barrier and provide a more objective look onto the systems under investigation[1]. Unfortunately, tools using this method are not widely available and often lack flexibilty. In this presentation we will demonstrate a Python software suite aiming at quickly developing script based models for further bayesian sampling. Special parametrization methods of the models based on concentration profiles rather than a description of the scattering length density will be shown to provide an intuitive and efficient fitting framework.

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Friday 12.10.17, 09:00-09:30

Revealing the nanoscale and interfacial behavior in complex magnetic systems at the ISIS spallation neutron source: current capabilities and future opportunities

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Quantifying the interfacial behavior of nanoscale magnetic systems is key to understanding a wide range of solid state physics phenomena. Moreover, such behavior often results in useful functional properties that can be exploited in devices. Spin diffusion lengths in ferromagnetic metals are typically much less than 100nm. This lengthscale gives an indication of the resolution required to spatially resolve interfacial physics such as: proximity magnetism, the spin-Seebeck effect, doped topological insulators and superconducting spintronics. Providing a quantitative understanding of such phenomena presents a significant experimental challenge. The interfaces of interest are often buried and not readily accessible to more conventional macroscopic techniques. Neutron techniques provide unparalleled quantitative access to such systems through the exploitation of polarized neutrons in reflection and small angle scattering geometries.

In this talk we shall introduce the capabilities of the current suite of polarized instrumentation at ISIS and highlight some of the recent science it has delivered. Examples will be taken from recent studies of topological matter [1-3], materials for magnonics [4], synthetic antiferromagnets [5] and thin film rare-earths [6] for spin triplet generation.

We shall also describe some of the possibilities for future instrumentation at the ISIS source.

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Friday 12.10.17, 09:30-10:00

Peculiarities of Time-of-Flight Grazing Incidence Neutron Scattering with Polarized Neutrons

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Grazing incidence neutron scattering (GINS) (specular reflection, off-specular scattering (OSS) and Grazing Incidence Small Angle Scattering (GISANS), establishes a direct and precise correlation between local interfacial characteristics and global physical properties and delivers the most exhaustive and detailed information on the 3-dimensional structure of thin films and hidden interfaces on enormous length scale.

At present, most of published data in reflectometry are obtained with specular reflectivity, from which the structural information perpendicular to the sample surface is obtained along the Q_z component of the wave vector transfer. However, functionality often arises at the mesoscale, where defects, interfaces, and non-equilibrium structures are formed [1], which cannot be resolved only by specular reflectivity alone.

Spallation neutron sources can deliver outstanding experimental conditions to perform *simultaneously* a combined measurement of specular reflection, OSS and GISANS [2]. Pilot experiments performed at the SNS will be presented that include: new generation of heterostructures based on integrating topological insulators (TIs) with conventional materials to induce ferromagnetic interactions with symmetry breaking at the interface [3], tunnel barriers in hybrid organic/metallic spin-valve structures, asymmetric block-copolymer/nanoparticle composite structures. The specific details will be presented.

Work supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, and the US Department of Energy, by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory.

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Friday 12.10.17, 10:00-10:15

Chirality effects in Rare-Earth Multilayers investigated by the analysis of full polarized neutron reflectometry maps

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The presence of chirality plays a crucial role in many different disciplines in science and is often the key to understand phenomena in nature. In the recent years the chirality effect has finally also caught a lot of intention in the field of magnetism, particularly, when it could be linked to the appearance of the Dzyaloshinskii-Moriya (DM) interaction.

Here we report about our investigations of this intriguing phenomena in rare-earth multilayer in whose the chirality can be tuned by the application of an external magnetic field. Polarized neutron refelctometry is the tool of choice to study the dependence on composition, temperature and magnetic field [1, 2]. The interplay of the RKKY and the Zeeman interactions helps here to reveal the anti-symmetric Dzyaloshinskii-Moriya interaction since the observed chirality is a fingerprint of the DM interaction resulting from the lack of the symmetry inversion at the interfaces. Recently it could be shown that the field induced chirality effect has an alternative mechanism where an induced non-homogeneous anisotropy modifies the observed chirality behavior. Careful analysis of the polarized neutron measurements with complete polarization analysis allows one to link the occurrence of the effect with changes in the magnetic structure. In the focus of this talk is the evaluation of full polarized scattering maps [3] allowing one to extract unique information of the mechanism behind the formation of the chirality effects in these systems.

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Friday 12.10.17, 10:45-11:00

Swelling and exchange kinetics in PNIPAM microgel thin films probed with in-situ neutron reflectometry

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Responsive materials show a strong change in one or multiple properties by a variation of an external stimulus. In this field, polymers are one of the most intensively studied materials due to their high variability and their large field of applications. Hydrogels, or in their colloidal form called microgels, are formed by crosslinking the polymers. Microgels exhibit new functionality and are of high interest for biomedical applications such as drug delivery and tissue engineering [1,2]. In order to gain detailed insights in the underlying processes the uptake and release of water, and the diffusion of the molecules through the interconnected network are of high interest.

Therefore, highly homogeneous microgel films constituted of PNIPAM homopolymer crosslinked with varying amounts of N,N'-methylenebisacrylamide are prepared. The films are pre-characterized with optical microscopy, atomic force microscopy and X-ray reflectometry. Different humidity conditions are applied at a constant temperature below the LCST of PNIPAM in a custom made chamber.

Neutron reflectometry in time of flight (TOF) mode is used to investigate the uptake and exchange kinetics of H_2O with D_2O and vice-versa in-situ. Different models for both, the swelling and exchange process are used to describe the release and uptake rate of the vapor phase into the polymer thin film [3,4]. Fourier transform infrared spectroscopy and white light interferometry are used to complement the collected data and prove the viability of the used models.

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Friday 12.10.17, 11:00-11:15

Small molecule profiles between lipid bilayers by neutron diffraction

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While well established for studying the internal structure of bilayers and orientation of peptides and proteins with respect to bilayers, neutron lamellar diffraction has a powerful inisght the average locus of solubilisation of small molecules in stacks of lipid bilayers[1-3]. The approach has provided unique insights into important issues in anhydrobiology and cryobiology, where previously only molecular dynamics simulations (MD) had been able to provide molecular scale insights. Currently we use the methodology to understand the interaction of cryoprotectants with bilayers, with the aim of providing important validation

of MD parameters to further enhance the utility of the method. Here we discuss the experimental approach, both in terms of the use of contrast variation and the use of selective deuteration to simplify the extraction of scattering length density profiles within the bilayer.

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Friday 12.10.17, 11:15-11:30

Neutron Scattering from Bio-Related Interfacial Structures: From Model Systems to Living Objects.

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Understanding structure and functionality of bio-related objects is important for broad range of applications: from innovative functionalized biomimetic materials to functions of complex biological systems. Due to non-perturbative nature, isotopic sensitivity and penetrability neutrons are well suited to study such systems. I will discuss neutron reflectivity and off-specular scattering studies of several bio-related interfacial structures in static conditions and under mechanical stress. One of the examples will cover the adhesion of living cells and their behavior under the external mechanical forces simulating the blood flow. Neutron reflectivity is very well established experimental tool for obtaining length-scale and density information about well-ordered, homogenous layered materials, such as *model* phospholipid bi- and mono-layers or polymeric thin films. It is more challenging to obtain any information about poorly stratified samples and samples that incompletely cover the surface. Measuring *living cells* adhesion provided a challenge due the complexity, inherent inhomogeneity of the system, a difficulty in controlling and producing samples with consistent surface coverage and *biological safety requirements*. However, understanding of the cell adhesion in dynamic conditions can be connected with mitigating atherosclerosis and understanding of migration of cancerous cells.

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Friday 12.10.17, 11:30-11:45

A simple, single-step procedure for the preparation of responsive surfactant-polysaccharide multilayered coatings

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The preparation of functional coatings which are able to trigger specific structural changes as a response to external stimuli has an increasing demand in many technologies. However, the design of simple methods, which allow fast and scaled-up sample preparation, remains a challenging task. Sequential layer-by-layer assembly of molecules onto solid surface has been largely established for the preparation of stimuli-responsive nanostructured films. While this method is extremely versatile in terms of number of employed materials, its application can be limited by the large number of steps required.

In this contribution, we present a new method to prepare multilayered polyelectrolyte – surfactant coatings on solid substrate with a single step procedure. In particular, we demonstrate that well-defined multilayered vesicles formed in bulk solution between the biopolycation chitosan and oppositely charged ethoxylated surfactants[1] can be transferred to a solid surface via spin-coating. The coatings retain the main structural features of their parent self-assemblies in bulk solution, such as layer thickness and number of layers. This strategy allows to control the structure of the adsorbed multilayers through the bulk self-assembly process in bulk prior to film deposition.

The structural characterization of the multilayered vesicles in bulk was performed by small-angle neutron scattering, while the morphology of the coatings was probed by neutron reflectometry under increasing humidity. The combined study demonstrate the formation of an ordered alternation of layers with responsive properties which can be tuned by small variations of the bulk self-assembly conditions prior to film deposition.

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Abstracts

Poster sessions

Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Artem FEOKTYSTOV	**KWS-1 for grazing incidence small-angle neutron scattering GISANS**
Artur Glavic	**Structure and Phase Transitions in Spontelectric Methylformate**
Emmanuel KENTZINGER	**Polarized GISANS from lateral correlations of the spin misalignment**
V.I.PETRENKO	**Optimization aspects in design of experiments on neutron reflectometry from electrochemical interfaces with liquid electrolytes**
Patrick SCHÖFFMANN	**Pre-characterization of thin film samples by atomic and magnetic force microscopy**
Annika STELLHORN	**Interactions between superconductor-ferromagnet thin films**
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Markus WASCHK	**Interface phenomena in $La_{1/3}Sr_{2/3}FeO_3$ / $La_{2/3}Sr_{1/3}MnO_3$ heterostructures**
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Senlin XIA	**Neutron reflectivity investigation on thermo-responsive copolymers with embedded magnetic nanoparticles**
Michaela Zamponi	**Upgrades of the backscattering spectrometer SPHERES**

Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

KWS-1 for grazing incidence small-angle neutron scattering GISANS

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The KWS-1 small-angle neutron scattering instrument is operated by Jülich Centre for Neutron Science (JCNS) and located at the research reactor FRM II of the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching. This is a highly flexible instrument with many possibilities and options available for users. Among them is the grazing incidence neutron scattering (GISANS) option which allows experiments on soft matter and magnetic thin films.

The needed slit collimation either in the vertical or in the horizontal direction is easily reached with active collimation apertures that allow arbitrary beam cross-section between 1x1 and 30x30 mm^2. A compact cradle, which allows tilting and rotating of the sample in the beam, is available for GISANS experiments with light sample environment. For heavy sample environment positioning, KWS-1 has a custom-designed hexapod at the sample position. The hexapod can carry around 550 kg of a useful load. The six feet of the hexapod allow flexible positioning and trajectories of the sample in all three spatial directions about an arbitrary point above the table of the hexapod, which is difficult to achieve by systems of several individual stepper motors. The hexapod can move in the range of 20 cm in the vertical Z direction and ±18 cm in the horizontal X and Y directions (this value strongly depends on the Z position). The hexapod was additionally mounted on a rotating table. Thus the Z rotation is limited practically only by cable length. As the hexapod is built exclusively from nonmagnetic materials, no shielding is necessary, even if it carries magnets with high magnetic fields. The high precision of the hexapod (0.01 mm and 0.01°) allows the investigation of magnetic nanoparticles deposited on substrates and thin films of nanostructured polymeric materials by GISANS with the additional application of magnetic field on the sample. Special adaptors allow the mounting of a 5 T vertical cryomagnet (300 kg) and a vertical electromagnet of 2.2 T (500 kg) on its table. The cryomagnet can provide a 3-300 K temperature range on the sample. The electromagnet can be equipped either with a temperature-controlled sample changer (from room temperature and higher) or with a cryofinger for temperatures in the range of 10-300 K. Both magnets are shielded, have weak stray fields, and are suited for experiments with polarized neutrons and polarization analysis.

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Structure and Phase Transitions in Spontelectric Methylformate

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Spontelectric materials are molecules of polar nature which, when deposited as thin films under the right vacuum and temperature conditions, can form spontaneous electric fields along the surface normal of the substrate. While these electric polarizations have been measured in several different materials and studied with optical spectroscopy and macroscopic methods, the underlying mechanism for the spontaneous alignment of the molecular dipoles is still purely understood. In methylformate, one of these spontelectric systems, several measurements point to changes in the structure after the film deposition, that may be related to a phase change to a crystalline order.

To investigate the nature of this phase transition and the structure during film growth in general, we have measured neutron reflectivity from methylformate thin films, deposited in-situ at the Magnetism Reflectometer beamline of SNS. We have employed magnetic contrast variation with platinum coated cobalt layers together with controlled deposition of various protonated and deuterated film sequences to become sensitive to various features of the films, including intra-layer diffusion and molecular density. We have found clear structural changes when annealing through the phase transition as well as a dependence of such changes on the deposition temperature, that correlate with changes in the electric polarization of these films.

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Polarized GISANS from lateral correlations of the spin misalignment

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Off-specular and grazing incidence small angle neutron scattering with polarization analysis from small magnetic objects on a substrate allow depth-resolved investigation of the lateral magnetic correlations at mesoscopic length scales [1].

In the past, we have simulated off-specular scattering of polarized neutrons from laterally patterned magnetic multilayers, based on the formalism developed by Boris Toperverg [2]. We would like to present how we used this theory so far [3].

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Optimization aspects in design of experiments on neutron reflectometry from electrochemical interfaces with liquid electrolytes

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Nowadays, Li-ion batteries are used to supply electrical devices from mp3 players to cars. The development of high-capacity rechargeable and safe metallic lithium negative electrodes for next-generation batteries depends on in-depth understanding of reasons for non-uniform lithium plating during lithium-metal battery charge. In its turn, it drives the interest to the tools enabling efficient monitoring of electrochemical interfaces where lithium electrodeposition occurs on electrode surfaces in contact with liquid electrolytes. Neutron reflectometry (NR) is one of the few methods suitable for operando studies of the evolution of electrochemical interfaces including the formation of solid-electrolyte interphase (SEI) and other kinds of deposition. A special cell is required for such type of experiments [1] which should satisfy several requirements with respect to liquid electrolyte and solid electrode in order to provide maximal sensitivity of the NR experiment to the changes at the interface. Thus, there is an optimization problem in the design of experiment concerning the parameters of the electrode/SEI/electrolyte interface.

The aim of the given work is to propose a protocol and choose the optimal parameters of the thin metal electrode and electrolyte type (including various deuteration rate of the liquid component) for the most effective operando NR studies of lithium-enriched electrodeposition. For this purpose, the formation of SEI and further lithium plating are modeled by calculating specular NR curves for various combinations of scattering length densities, thicknesses and width of the interlayered transitions in the depth interface profile including the cases of complex electrode structures.

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Pre-characterization of thin film samples by atomic and magnetic force microscopy

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Atomic force microscopy (AFM) is a scanning probe microscopy technique for the investigation of the surface topography. A tip is scanned above the sample in close or direct contact with the surface and interacts with the sample mainly via van-der-Waals and chemical forces. Mostly, the tapping mode is used, where the cantilever oscillates close to its resonant frequency and the tip-sample interaction changes the resonance frequency, amplitude and phase of the oscillation. The topography is visualized by recording the adjustment of the tip-sample distance which is necessary to keep the amplitude constant.

Magnetic force microscopy (MFM) uses a magnetic tip for a similar scan but probes the interaction of the tip with the magnetic stray field of the sample at a higher distance from the sample to exclude the topographic information. The change in the magnetic stray field perpendicular to the sample surface is detected as a phase change of the cantilever oscillation.

An Agilent/Keysight 5500 SPM is available for MFM and AFM measurements in the thin film laboratory at JCNS@MLZ, for room temperature use. The lateral resolution of the AFM is about 10 nm while the vertical resolution amounts to 0.4 nm.

As an example, we will present the evolution of the magnetic structure of a $[FePt/Fe]_6/MgO$ multilayer system prepared by molecular beam epitaxy for different Fe film thicknesses. For an Fe layer thickness of 1 nm the magnetic stray field forms a maze pattern with closed-of bubbles and no preferential direction. With increasing Fe thickness the domains begin to form increasingly longer, but still branching stripes, with a clear preferential direction, and a decrease in the amount of local, disordered structures and bubbles.

MFM can be used as a pre-characterization tool for neutron measurements to investigate the real-space magnetic structure of the surface and to orient thin film samples with a magnetic pattern relative to the neutron beam direction for the measurement in neutron reflectometry and SANS instruments, e.g. MARIA and KWS-3. Additionally, it may be of interest to compare the magnetic structure before and after the measurement in a magnetic field.

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Interactions between superconductor-ferromagnet thin films

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Ferromagnetism and superconductivity have long been considered as antagonist phenomena. When the magnetic state of the ferromagnet is inhomogeneous, magnetic domains and domain walls can guide the vortices and spatially confine the superconductivity in an adjacent superconducting layer [1]. Additionally new physical phenomena like the proximity effect occur at the interface between a superconductor and an inhomogeneous ferromagnet. On the application point of view, superconductor-ferromagnet thin films may lead to great improvements in spintronics [2]. Due to the perpendicular magnetic anisotropy and a periodic magnetic field distribution of FePd thin films, this structure can be used in bit-patterned media.

Our goal is to obtain an understanding of the proximity effect occurring between ferromagnetic thin films and superconducting layers. We want to investigate the effect of different magnetic domain structures of the ferromagnet onto a superconducting toplayer and vice versa, as well as the influence on the superconducting critical temperature.

As prototype system we use ferromagnetic FePd thin films with a toplayer of Nb as superconductor grown by Molecular-Beam-Epitaxy (MBE). To gain epitaxial growth the FePd is deposited on a buffer layer of Pd and Cr on a MgO substrate [3]. Deposited below 600°C, FePd grows in the L10-ordered phase with a magneto-crystalline anisotropy perpendicular to the surface plane with stripe-shaped domains.

To investigate in particular the depth profile of the magnetic domain structure we use Grazing-Incidence-Small-Angle-Neutron-Scattering (GISANS). The characterization of the macroscopic magnetization is performed with superconducting quantum interference detector (SQUID)-measurements. Furthermore the crystallography and layer thicknesses are measured with X-ray scattering, whereas the composition of the FePd compound layers are characterized with Rutherford Backscattering (RBS).

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Spin dependent giant junction resistance in Fe/p-Si Schottky heterojunction

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With a motivation to find a simple magnetoresistive device which could show appreciably large change in its electrical conductance with application of small magnetic field and at a relatively low bias voltage (thereby reducing the heat dissipation in the system), in this work we report on a giant positive magnetoreistive behavior of a simple Fe/p-Si Schottky heterojunction diode at low temperatures.

The device shows good rectifying characteristics at room temperature and a dual - Schottky as well as magnetic diode - characteristics at low temperature, below 50 K. Formation of a magnetic field dependent potential barrier at the interface, due to electrical injection of spin-polarized carriers from the ferromagnetic electrode into the semiconductor template [1-4], is referred to result in such large junction resistance.

The quantitative analysis of the field dependence of the Fe/p-Si diode characteristics at low temperature, reveal a spin diffusion length of 100 nm with a spin life-time 300 ps. The magnetoresistance value is of the order of 10^4% at 10 K and saturates at a much lower magnetic field (~0.5 kOe), thus making it a better choice for magnetic diode as well as magnetoresistive device.

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Tuesday, 10.17.2017 and Wednesday 11.10.2017, 16:30-18:00

Interface phenomena in $La_{1/3}Sr_{2/3}FeO_3$ / $La_{2/3}Sr_{1/3}MnO_3$ heterostructures

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Transition metal oxides (TMO's) exhibit electronic correlations and complex ordering phenomena which make them ideal candidates for sensors and storage devices in future information technology. Such devices will consist of heterostructures of different TMO's, where interfaces can add functionalities, which cannot be found in the individual constituents. The subtle balance between electronic, spin, and lattice degrees of freedom leads to a variety of quantum phenomena and results in an extreme sensitivity to external stimuli such as pressure and magnetic fields. Especially the interface between two materials in a heterostructure can exhibit completely new phenomena due to the reduced dimensionality and epitaxial strain, for instance. An interesting system is the heterostructure $La_{1/3}Sr_{2/3}FeO_3$ / $La_{2/3}Sr_{1/3}MnO_3$ (LSFO / LSMO). LSFO contains a Verwey transition with a resistivity increase of eight orders of magnitude from 300 K to 10 K, coinciding with an antiferromagnetic and charge ordering transition. In contrast, LSMO is a ferromagnetic conductor. Thus, this heterostructure is an ideal candidate to study the interfacial coupling and electronic doping effect of both materials with regard to effects on the magnetization of LSMO within the interface. High quality heterostructures were grown with a combination of a state-of-the-art oxide molecular beam epitaxy system and a sputtering technique and subsequently analyzed with a SQUID magnetometer as well as polarized neutron reflectometry (PNR) and scanning transmission electron microscopy (STEM). The interface morphology, and thus the magnetic properties within the interface region, depends crucially on the growth order. STEM shows significant iron interdiffusion from pre-deposited LSFO into the LSMO layer to at least nine unit cells is observable for the LSMO/LSFO, whereas the LSFO deposited on LSMO exhibits a sharp interface with interdiffusion restricted to two unit cells at most. The differences in the interface morphology for different growth orders also affects the magnetic properties and the coupling between both single layers. The LSMO/LSFO sample shows an increased Curie temperature, a reduced interface magnetization, and a vanishing exchange bias effect. In contrast, the system LSMO/LSFO has a homogeneous magnetization in the whole LSMO layer, but the macroscopic magnetization measurements reveal an additional magnetic impurity phase which persists also at high temperatures. Additionally, M(H) measurements feature an inverted hysteresis and a strong field cooling dependency of magnetization, which includes a significant exchange bias effect.

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Towards neutron scattering experiments with sub-millisecond time resolution

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Neutron scattering techniques offer several unique opportunities in materials research. However, most neutron scattering experiments suffer from the limited flux available at current facilities. This limitation becomes even more severe if time-resolved or kinetic experiments are performed. A new method has been developed which overcomes these limitations when a reversible process is studied, without any compromise on resolution or beam intensity. It is demonstrated that, by recording in absolute time the neutron detector events linked to an excitation, information can be resolved on sub-millisecond timescales. Specifically, the concept of the method is demonstrated by neutron reflectivity measurements in time-of-flight mode at the Liquids Reflectometer located at the Spallation Neutron Source, Oak Ridge National Laboratory, Tennessee, USA, combined with *in situ* rheometry. The opportunities and limitations of this new technique are evaluated by investigations of a micellar polymer solution offering excellent scattering contrast combined with high sensitivity to shear.

[1] F. A. Adlmann, P. Gutfreund, J. F. Ankner, J. F. Browning, A. Parizzi, B. Vacaliuc, C. E. Halbert, J. P. Rich, A. J. C. Dennison, M. Wolff, J. Appl. Cryst. **48**, 220 (2015).

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Using wave field enhancement to enable inelastic scattering studies of hydrogen diffusion in thin films

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Surface sensitive neutron scattering techniques are often limited by the relatively low brilliance of neutron sources. This makes gracing incidence neutron scattering studies challenging and is even more limiting if one is interested in diffusion processes and quasielastic scattering. One way to overcome this challenge is to use wave field enhancement in a potential well. Recently, such methods have been implemented to study dynamics in liquids near a solid interface by neutron spin echo methods [1-3]. Here we present an alternative approach of hydrogen diffusion in thin films of vanadium. The main difference to the experiments mentioned above is that in our case the hydrogen diffuses in the resonating layer allowing better control of the neutron wave field. Vanadium has a small scattering cross section and can take up hydrogen in large quantities. Moreover, thin layers of vanadium show profound finite size, proximity and confinement effects [4]. Considering this these sample systems offer an ideal test case to push the current limits regarding inelastic neutron scattering experiments from thin films.

In this presentation the recent results from a 100 nm V resonator layer will be presented. We show that the incoherent scattering from the hydrogen is detectable but only slightly above the background level. Opportunities and challenges of the method regarding optimized samples as well as instrument setups will be discussed.

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[2] Jaksch, S., Lipfert, F., Koutsioubas, A., Mattauch, S., Holderer, O., Ivanova, O., Frielinghaus, H., Hertrich, S., Fischer, S.F., Nickel, B. Phys. Rev. E **91**, 022716 (2015).

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Neutron reflectivity investigation on thermo-responsive copolymers with embedded magnetic nanoparticles

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Nanostructured thin films with embedded magnetic nanoparticles (NPs) are promising in magnetic applications due to their novel chemical and physical properties. The realization of desired magnetic properties depends on the arrangement of the NPs and can be tuned by employing diblock copolymers as host matrixes. Various ordered nanostructured templates can be achieved from the phase separation of diblock copolymers composed of two chemically incompatible blocks. Being coated with one particular type of polymer chains, magnetic NPs can have a selective affinity to one of the blocks and get well distributed within this domain [1]. So far, thermo-responsive copolymers are rarely investigated as host materials for magnetic NPs despite of their high potential.

Recently, we investigated the nanostructure and magnetic behavior of hybrid dry films consisting of magnetite (γ-Fe_2O_3) NPs coated with polystyrene chains and the diblock copolymer polystyrene-block-polyN-isopropylacrylamide (PS-b-PNIPAM) [1]. Results showed selective incorporation of NPs into the PS domains and a morphological evolution from parallel cylinders to perpendicular ones at low NP concentrations. A superparamagnetic behavior was found irrespective of the NP concentration. Since PS-b-PNIPAM films are most interesting under wet conditions, we extend our investigation from dry films to wet ones in order to explore the swelling behavior of the hybrid films and its impact on the magnetic properties. Neutron reflectivity is used to detect the morphology of hybrid films as a function of temperature in a humid atmosphere. In addition, polarized neutron reflectivity is used to probe the magnetic structure of the PS-b-PNIPAM films with magnetite NPs.

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Upgrades of the backscattering spectrometer SPHERES

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The neutron backscattering spectrometer SPHERES (SPectrometer for High Energy RESolution) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It provides high energy resolution of about 0.66μeV with a good signal-to-noise ratio [1]. 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. So is it possible for example to see how polymer dynamics is affected by nanoscopic confinement [2] or follow the dynamics of water confined in porous material [3].

Recently the PST chopper has been upgraded. Together with the exchange of the chopper also the graphite deflector crystals on its circumference were replaced with ones of a higher reflectivity and mosaicity. The new more compact one-wing chopper can be operated with the desired frequency with a crystal speed of 225m/s close to the optimum velocity for the phase space transformation. Thanks to the increased velocity and the better deflector crystals, the intensity in most detectors has been doubled.

Further improvement of the instrument performance is expected from the planned upgrade of the focusing neutron guide and the introduction of a background chopper. The focusing guide has been optimized for higher flux and low background based on simulations which also consider the new PST chopper. With the new elliptic guide an intensity gain at the sample position of about 40% is expected. Together with the exchange of the focusing guide also a background chopper will be incorporated to further reduce background and to allow for an increased signal-to-noise ratio setup by eliminating every second pulse, albeit at the cost of intensity.

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Location and Accommodation

The workshop venue is the ideally-located Conference Center of the Evangelische Akademie Tutzing, situated directly on Lake Starnberg in the foothills of the Alps, approximately 40km south of Munich.

The workshop fee includes accommodation for 3 nights (10-13 October), fullboard and the workshop dinner.

Accommodation is in single rooms. If the number of participants exceeds the number of rooms available in the Evangelische Akademie, equivalent accommodation will be organized in hotels in Tutzing. These hotels are all within short walking distance of the Akademie.

How to reach Tutzing

From the center of Munich (approx. 50 minutes)

• At Munich main station take the S6 (leaves every 20 minutes) in the direction of Tutzing.
• From the S-Bahn station in Tutzing it is within 10 min walking to the Evangelische Akademie at the lake Starnberg.

From Munich airport (approx. 90 minutes)

• If your flight ticket does not include a journey in the MVV area, your journey on the S-Bahn (city train) to Tutzing requires a day ticket for the external area (Außenraum).
• Take the S1 (eaves every 20 min) in the direction of Munich Hauptbahnhof (main station) as far as Laim station (approx. 40 minutes)
• At Laim change trains at the same platform for the S6 to Tutzing.
• The Evangelische Akademie is approx. 10 min walking distance from the S-Bahn station Tutzing at the lake Starnberg.

You can find information on the trainor bus schedule at the webpage of the Munich Public Transportation Service

http://www.mvv-muenchen.de/en/homepage/index.html

or the Deutsche Bahn service

http://www.bahn.de/p_en/view/index.shtml

List of partcipants