

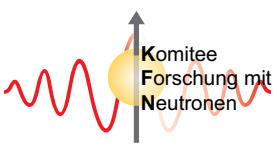
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German Neutron Scattering Conference

Deutsche Neutronenstreutagung 2012

September 24 - 26, 2012

Gustav-Stresemann-Institut, Bonn, Germany



Forschungszentrum Jülich GmbH
Jülich Centre for Neutron Science
Peter Grünberg Institute

German Neutron Scattering Conference

Deutsche Neutronenstreutagung 2012

September 24 – 26, 2012
Gustav-Stresemann-Institut, Bonn, Germany

Programme and Abstracts

Thomas Brückel (Editor)

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German Neutron Scattering Conference Deutsche Neutronenstreutagung 2012

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Supported by: Forschungszentrum Jülich GmbH
German ESS-DU
Helmholtz-Zentrum Berlin
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Organized by: „Jülich Centre for Neutron Science“
for “Komitee Forschung mit Neutronen”



German Neutron Scattering Conference
Deutsche Neutronenstreutagung 2012
September 24 - 26, 2012

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German Neutron Scattering Conference
Deutsche Neutronenstreutagung 2012
September 24 - 26, 2012

Invited Speakers

Hartmut Abele	<i>Universität Wien, Austria</i>
Manuel Angst	<i>Forschungszentrum Jülich GmbH, Germany</i>
Dimitri Argyriou	<i>ESS, Sweden</i>
Stephan Förster	<i>Universität Bayreuth, Germany</i>
Raphaël Hermann	<i>Forschungszentrum Jülich, Germany</i>
Holger Kohlmann	<i>Universität des Saarlandes, Germany</i>
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Christian Pfleiderer	<i>Technische Universität München, Germany</i>
Harald Schmidt	<i>Technische Universität Clausthal, Germany</i>
Torsten Soldner	<i>Institut Laue-Langevin, France</i>
Alan Tennant	<i>Helmholtz-Zentrum Berlin, Germany</i>
Andreas Wischnewski	<i>Forschungszentrum Jülich GmbH, Germany</i>

Welcome to Bonn and DN 2012

The German Neutron Scattering Conference 2012 – Deutsche Neutronenstreutagung DN 2012 offers a forum for the presentation and critical discussion of recent results obtained with neutron scattering and complementary techniques. The meeting is organized on behalf of the German Committee for Research with Neutrons – Komitee Forschung mit Neutronen KFN – by the Jülich Centre for Neutron Science JCNS of Forschungszentrum Jülich GmbH. In between the large European and international neutron scattering conferences ECNS (2011 in Prague) and ICNS (2013 in Edinburgh), it offers the vibrant German and international neutron community an opportunity to debate topical issues in a stimulating atmosphere. Originating from “BMBF Verbundtreffen” – meetings for projects funded by the German Federal Ministry of Education and Research – this conference series has a strong tradition of providing a forum for the discussion of collaborative research projects and future developments in the field of research with neutrons in general. Neutron scattering, by its very nature, is used as a powerful probe in many different disciplines and areas, from particle and condensed matter physics through to chemistry, biology, materials sciences, engineering sciences, right up to geology and cultural heritage; the German Neutron Scattering Conference thus provides a unique chance for exploring interdisciplinary research opportunities. It also serves as a showcase for recent method and instrument developments and to inform users of new advances at neutron facilities.

We are grateful for the financial support from the neutron centres FZJ, HZB, HZG, ILL, TUM and the German ESS-Design update project, which allows us to support the participation of young scientists and to award the prestigious “Wolfram-Prandl Prize”.

The German and European neutron communities are eagerly looking forward to the realization of the European Spallation Source ESS in Lund, Sweden. With a beam power of 5 MW, this novel long pulse source will lead neutron scattering into a new era and enable scientists to perform experiments that they can only dream of today. The German neutron community, being one of the largest and most productive worldwide, is keen to contribute to the future realization and scientific exploitation of this leading source. Special sessions will be dedicated to explore how this next-generation neutron facility can best contribute to solving the Grand Challenges modern societies face in terms of energy, information technology, transport, health and the environment.

Enjoy the conference and your time in Bonn!

Thomas Brückel
- for the organizers -

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Programme

**German Neutron Scattering Conference/
Deutsche Neutronenstreutagung 2012**
Gustav-Stresemann-Institut (GSI), Bonn, Germany

Time	Monday, September 24, 2012	
09:00 – 11:00 h	Registration	
11:00 – 11:15 h	Welcome: Th. Brückel and T. Unruh	
11:15 – 12:30 h	Hydrogen Chemistry and Energy (Chairman: R. Dronskowski)	
PT01	<u>H. Kohlmann</u>	<i>Watching metal hydride formation in situ</i>
CT01	<u>M. Skoda</u>	Hydrogen absorption in Mg-Ti multilayers studied by neutron reflectometry
CT02	<u>K. Pranzas</u>	NCT and SANS investigations of hydrogen tanks and solid state hydrogen storage materials
CT03	<u>A. Senyshyn</u>	Neutron powder diffraction and “green” energy challenges
12:30 – 14:00 h	LUNCH	
14:00 – 15:30 h	Material Science (Chairman: A. Schreyer)	
PT02	<u>H. Schmidt</u>	<i>Atomic diffusion in solids - Experiments with neutron reflectometry</i>
CT04	<u>M. Karg</u>	Gold nanocrystal superlattices: A small angle neutron scattering study
CT05	<u>E. Josten</u>	Structural and magnetic correlations in 3D ordered nanoparticle assemblies
CT06	<u>F. Kargl</u>	Diffusion properties of metallic liquids and their binary alloys
CT07	<u>D. Holland-Moritz</u>	Neutron scattering experiments on Zr-based melts processed by electrostatic levitation
15:30 – 16:00 h	COFFEE	
16:00 – 19:00 h	Poster Session	
19:00 h	DINNER	
20:00 h	Poster Session (continued with beverages)	

**German Neutron Scattering Conference/
Deutsche Neutronenstreutagung 2012
Gustav-Stresemann-Institut (GSI), Bonn, Germany**

Time	Tuesday, September 25, 2012	
09:00 – 10:30 h PT03 CT08	Magnetism I A. <u>Tennant</u> F. <u>Weber</u>	(Chairman: M. Loewenhaupt) <i>tba</i> Electron-phonon coupling in the conventional superconductor YNi ₂ B ₂ C at high phonon energies studied by time-of-flight neutron spectroscopy
CT09	A. <u>Hiess</u>	Chirality of the spin resonance in the unconventional superconductor CeCoIn ₅ investigated with polarized neutrons under magnetic field
CT10	A. <u>Walters</u>	A neutron resonance spin-echo study of the symmetry of the order parameter in an iron-based superconductor
CT11	S. <u>Krannich</u>	Spin fluctuations and phonon softening in the strongly correlated semiconductor FeSi
10:30 – 11:00 h	COFFEE	
11:00 – 12:30 h PT04 CT12	Soft Matter S. <u>Förster</u> H. <u>Morhenn</u>	(Chairman: M. Gradzielski) <i>Structure of soft lyotropic crystals and quasicrystals</i> The motions in liquid n-alkanes: A neutron scattering and MD simulations study
CT13	P. <u>Müller-Buschbaum</u>	Phase separation and molecular intermixing in polymer-fullerene bulk heterojunction thin films
CT14	I. <u>Hoffmann</u>	Dynamics and structure of polyelectrolytes in aggregates with oppositely charged surfactants
CT15	M. <u>Appel</u>	Ring rotation dynamics of ferrocene and ferrocene-containing polymers
12:30 – 14:00 h	LUNCH	
14:00 – 15:00 h PT05 CT16	Advanced Methods T. <u>Soldner</u> H. <u>Frielinghaus</u>	(Chairman: P. Fierlinger) <i>Precision measurements with cold neutrons</i> Dynamics of microemulsions adjacent to planar hydrophilic walls
CT17	W. <u>Treimer</u>	Quantum mechanical effects in superconductors visualized and quantified with polarized neutrons
15:00 – 16:00 h PT06 PT07 PT08	ESS Session I D. <u>Argyriou</u> A. <u>Wischniewski</u> H. <u>Abele</u>	(Chairman: T. Unruh) <i>Scientific Strategy for the European Spallation Source (15')</i> <i>The German contribution to the ESS Design Update Phase (15')</i> <i>Spectroscopy of Gravity</i>
16:00 – 16:30 h	COFFEE	
16:30 – 18:00 h PT09 PT10 PT11	ESS Session II R. <u>Hermann</u> T. <u>Nylander</u> C. <u>Pfleiderer</u>	(Chairman: Th. Brückel) <i>Neutrons and Energy materials: Present research and future opportunities</i> <i>Providing insight on bio-molecular interactions with biological membranes by using neutron scattering techniques - challenges and outlook</i> <i>Emergent phenomena of complex electronic materials</i>
18:00 – 19:00 h PT12	Wolfram-Prandl Prize NN	<i>Wolfram-Prandl Prize lecture</i>
19:30 h 20:00 h 22:30 h	Bus transfer CONFERENCE DINNER Bus transfer	GSI - Godesburg Godesburg Godesburg - GSI

**German Neutron Scattering Conference/
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Gustav-Stresemann-Institut (GSI), Bonn, Germany

Time	Wednesday, September 26, 2012	
09:00 – 10:30 h	Health and Life	(Chairman: Th. Hellweg)
PT13	B. <u>Nickel</u>	<i>Asymmetry and phase separation in lipid membranes</i>
CT18	F. <u>Schreiber</u>	Phase behaviour and associated dynamics of protein solutions manipulated by ions
CT19	T. <u>Nawroth</u>	Bio-nanoparticles for medical applications, enhancer radiotherapy - SANS, DLS & ASAXS
CT20	A. <u>Stadler</u>	Thermal fluctuations of haemoglobin from different species: Adaptation to temperature via conformational dynamics
CT21	M. <u>Schmiele</u>	Small angle scattering study on the stabilizer layer in triglyceride suspensions
10:30 – 11:00 h	COFFEE	
11:00 – 12:30 h	Information Technology and Magnetism II	(Chairman: G. Roth)
PT14	M. <u>Angst</u>	<i>Multiferroicity from charge ordering? A case study</i>
CT22	D. <u>Lott</u>	Chirality effects in rare-earth multilayers investigated by polarized neutrons
CT23	D. <u>Greving</u>	Magnetic correlations in dipolarly coupled iron oxide monolayer and multilayer films
CT24	V. <u>Zhernenkov</u>	RF field stimulated magnetization kinetics probed in thin films with MIEZE based Time-Resolved AC (TRAC) PNR
CT25	M. <u>Loewenhaupt</u>	Low-energy and crystal field excitations in single-crystalline CeCu ₂ Ge ₂ in fields up to 12 T
12:30 – 14:00 h	LUNCH	
14:00 – 15:30 h	Instrumentation	(Chairman: J. Neuhaus)
CT26	F. <u>Groitzl</u>	Larmor labeling methods: Neutron resonance spin echo spectroscopy beyond standard line width measurements
CT27	A. <u>Radulescu</u>	KWS-2 – the high-intensity / wide Q-range small-angle neutron diffractometer with tunable resolution at the FRM II optimized for soft-matter and biology
CT28	P. <u>Lindner</u>	Recent developments in sample environment for SANS at D11@ILL
CT29	E. <u>Babcock</u>	Polarization analysis with ³ He spin filters to separate coherent scattering from total scattering in SANS
CT30	W. <u>Kreuzpaintner</u>	In-situ neutron reflectometry during thin film growth by sputter deposition
CT31	F. <u>Mezei</u>	Neutron generation and beam extraction at ESS
15:30 – 16:00 h	CLOSING	

PT invited lectures 30 minutes total
CT contributed talk 15 minutes total

Talks

Talks Monday, September 24, 2012

PT01 *H. Kohlmann*

Watching metal hydride formation in situ

CT01 *M. Skoda*

Hydrogen absorption in Mg-Ti multilayers studied by neutron reflectometry

CT02 *K. Pranzas*

NCT and SANS investigations of hydrogen tanks and solid state hydrogen storage materials

CT03 *A. Senyshyn*

Neutron powder diffraction and “green” energy challenges

PT02 *H. Schmidt*

Atomic diffusion in solids - Experiments with neutron reflectometry

CT04 *M. Karg*

Gold nanocrystal superlattices: A small angle neutron scattering study

CT05 *E. Josten*

Structural and magnetic correlations in 3D ordered nanoparticle assemblies

CT06 *F. Kargl*

Diffusion properties of metallic liquids and their binary alloys

CT07 *D. Holland-Moritz*

Neutron scattering experiments on Zr-based melts processed by electrostatic levitation

PT01

Watching metal hydride formation *in situ*

H. Kohlmann, N. Kurtzemann, C. Reichert and P. Wenderoth

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Hydrogen chemistry and energy research are closely linked together in the field of metal hydrides, which are of great interest as potential hydrogen storage media. Solving the storage problem for hydrogen is considered to be one of the key issues for realizing a hydrogen based economy [1, 2]. Structural studies on such metal-hydrogen systems rely heavily on neutron diffraction. A variety of examples, ranging from ambient conditions to low temperature and high pressures, demonstrate the capability of state of the art neutron science [3, 4].

For a deeper understanding of the basic steps of the formation of and the hydrogen release from metal hydrides – the key steps in reversible hydrogen storage – *in situ* investigations are indispensable. In order to collect high quality data on such solid-gas reactions, a gas pressure cell, based on a single crystal sapphire tube as a sample holder [5], was constructed for *in situ* neutron powder diffraction [6]. The potential of this *in situ* neutron diffraction technique will be demonstrated by various examples, e. g. a very detailed picture of the $\alpha \rightarrow \beta$ transition in palladium deuteride, hydrogen induced transformations in palladium rich intermetallics [6, 7] and metal hydride formation in light-weight intermetallics and Zintl phases. The combination with other *in situ* methods, such as thermal analysis [6] or X-ray diffraction [8], gives new insights into the reaction pathways of solid-gas reactions and may help the rational synthesis planning of hydrogen storage materials in the future.

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CT01

Hydrogen absorption in Mg-Ti multilayers studied by neutron reflectometry

**M.W.A Skoda¹, C. J. Kinane¹, R. Fan¹, S. Langridge¹, W. I. F. David¹,
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Mg-Ti thin film alloys have large H-storage capacities, fast kinetics of hydrogen absorption and desorption and are structurally stable. These qualities stem from a short-range ordered distribution of the Mg and Ti atoms. In order to study the influence of short-range order on the hydrogen sorption properties of Mg-Ti systems, we artificially engineered chemical segregation by depositing a Ti/Mg multilayer with 10 repetitions of Ti(2 nm)/Mg(4.4 nm). On exposure to H₂ a two-step hydrogenation process occurs with the Ti layers forming the hydride before Mg. In-situ, time resolved Neutron Reflectometry (NR) allows an accurate determination of the out-of-plane expansion associated with each hydrogenation step. The volume expansion expected for the hydrogenation of both Ti and Mg is transferred completely in the vertical direction, indicating that large plastic deformations have to occur upon hydrogen absorption. Owing to the large negative neutron scattering length of hydrogen, NR proves to be an excellent technique for the in-situ characterization of the hydrogen absorption properties of thin films.

CT02

NCT and SANS Investigations of Hydrogen Tanks and Solid State Hydrogen Storage Materials

**P. K. Pranzas¹, F. Karimi¹, S. Börries¹, F. Beckmann¹, O. Metz¹,
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T. Klassen¹ and A. Schreyer¹**

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Hydrogen is one of the most interesting vectors for renewable energy sources regarding storage, transport and conversion of energy for the future, especially for mobile applications. Reactive Hydride Composites (RHCs) are very promising solid state hydrogen storage materials due to high hydrogen densities, stability and safety. The hydrogen sorption kinetics of RHCs is distinctly improved by high-energy ball milling and the addition of suitable metal-based additives [1].

Hydrogen tanks filled with metal hydride powder or pellets were investigated using Neutron Radiography (NR) and Neutron Computerised Tomography (NCT) with thermal and very fast neutrons. Changes in the powder structure were characterized as well as the hydrogen distribution in the tank volume. A special tank for in situ NR and NCT experiments, "Flexistore", was developed at HZG, certified for pressures up to 150 bar and temperatures up to 400°C. With Flexistore in situ hydrogen sorption studies can be performed varying the parameters temperature, pressure and metal hydride material. The obtained information about hydrogen distribution and powder bed stability is necessary to optimize the compact tank design, the capacity and the heat transfer inside the tank volume.

Furthermore, small-angle neutron scattering (SANS) was used to study the nanostructure of the hydrogen containing metal hydride matrix in nanocrystalline RHC-systems. This is essential for the understanding of the various sorption processes and possible rate limiting processes in metal hydrides and helps in the development and further optimisation of this new type of hydrogen storage materials.

References

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CT03

Neutron powder diffraction and “green” energy challenges

**A. Senyshyn¹, M. Hoelzel¹, H. Boysen², M. Mühlbauer^{1,3}, O. Dolotko^{1,3},
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The rapid technology progress, whose consequences we can see and use in the every day life, is directly proportional to the amount of energy available to meet the growing demands of individuals and industries throughout the world. The major part of available energy is received from non-renewable sources and it is usually harmful to the environment upon burning. Thus, in the world energy production fossil fuels, like natural gas and crude oil, along with nuclear consist about 80% of the worldwide amount, which slowly drives the world towards the resources and ecology crisis and a single way to overcome the crisis safely is to find alternatives. This is the primary goal for modern science and, therefore, many research groups from science and industry are engaged into alternative energy research.

Nowadays the most of “green” (non-mechanical) energy applications are based anyhow on the light elements (hydrogen, lithium, oxygen), whose studies by conventional laboratory methods are quite challenging, i.e. desired detailing and accuracy can be hardly achieved. In this sense neutron scattering due to its unique features is an excellent tool, often having no alternative, when characterization of complex systems containing light elements, especially in the presence of heavy ones, is under discussion. The high penetration depths of thermal neutrons along with their low energy suit perfectly for non-destructive *in-situ* and *in-operando* studies of different kinds; the capability to localize light elements/isotopes (e.g. hydrogen, lithium) and to distinguish neighbouring elements from Periodic Table provides excellent phase contrast; the neutron scattering lengths not dependent on momentum transfer give accurate structure factors leading to precise bond-length and Debye-Waller factor analysis along with exact determination of diffusion pathways. On the other hand the high penetration depth of thermal neutrons along with the presence of either nearly neutron-transparent or nearly fully neutron-absorbing materials make the use of complicated sample environment (temperature, pressure, electric and magnetic fields, gas atmosphere, tension *etc.*) and its effect on the experimental results much simpler to account for.

In the current contribution a review of “green” energy-related scientific activities performed at the high-resolution neutron powder diffractometer SPODI at research reactor FRM-II will be presented with partial concern on modern thermoelectrics, materials for hydrogen storage, fast oxygen conductors for solid oxide fuel cells applications, electrode materials for enhanced lithium transport, Li-ion batteries *etc.*

PT02

Atomic Diffusion in Solids Experiments with Neutron Reflectometry

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Self-diffusion of atoms in solids is a fundamental point-defect mediated matter transport process. It plays a key role for the design and optimization of materials as well as for the performance of devices in various branches of technology like energy storage, electronic devices, sensor technology and nanostructural materials design.

The investigation of diffusion processes on very short lengths scales ranging from atomic distances up to some tens of nanometers is an emerging field of research. It is especially important for the characterization of nanostructured materials, metastable compounds and thin films as well as for the study of diffusion process close to room temperature.

During the talk, experiments are presented which are based neutron reflectometry applied to isotope multilayers [1,2]. This method detects the destruction of an artificial lattice of stable isotopes by thermally induced interdiffusion and enables to measure diffusion length down to some Angstroms.

Examples of recent research activities are presented for various classes of materials: Li ion conductors [5], elemental semiconductors [3] and nano-crystalline metallic films [4]. The advantages and further development of the method is discussed.

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CT04

Gold Nanocrystal Superlattices: A Small Angle Neutron Scattering Study

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The assembly of metal nanoparticles into superstructures with mm or even cm dimensions is a challenging scientific task. Despite the large quantity of monodisperse nanoparticles needed, the loss of colloidal stability is a major limitation to be overcome if such mesoscopic assemblies are of interest.

We coated gold nanocrystals with homogeneous cross-linked polymer shells resulting in core-shell hybrid particles with well-defined structures [1]. The polymer shells are composed of poly-*N*-isopropylacrylamide (PNIPAM), which is a thermoresponsive material. Due to the addition of this polymer shell, the effective particle volume of the nanoparticles is increased significantly. This allows reaching large particle volume fractions with a comparably low particle number.

Crystallization of these hybrid particles was observed over a broad range of particle concentrations at (and below) room temperature. Upon an increase in temperature, the PNIPAM shells shrink and the overall particle volume fraction decreases. This causes melting of the crystals in a certain concentration range. Upon cooling, crystallization occurs again, once a critical volume fraction is reached. These melting/recrystallization processes were observed to occur with very high reproducibility as will be demonstrated in this contribution.

Structural insights of the superlattices were obtained using Small Angle Neutron Scattering (SANS). In the low concentration regime, where inter-particle interactions can be neglected, the particle form factor $P(Q)$ was determined. In contrast, the scattering profiles for crystalline samples contain information on $P(Q)$ as well as on the structure factor $S(Q)$. Scattering profiles were recorded and analyzed for a broad range of concentrations and a variety of temperatures to study the phase behavior of the superlattices.

References

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CT05

Structural and magnetic correlations in 3D ordered nanoparticle assemblies

**E. Josten¹, U. Rücker¹, S. Mattauch¹, A. Glavic¹, A. Klapper¹,
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E. Brauweiler-Reuters⁴, D. Meertens⁵, E. Wetterskog⁶,
G. Salazar-Alvarez⁶, L. Bergström⁶ and Th. Brückel¹**

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Self-assembled systems of nanoparticles are candidates for new generation magnetic data storage media [1] or novel materials with tunable magnetic, optical or electronic properties [2,3]. Understanding the magnetic behavior of ordered nanoparticle arrays is an important step towards the controlled design of e.g. novel devices. We have studied γ -Fe₂O₃ nanocubes and nanospheres with a diameter ≈ 10 nm. Both types of nanoparticles show a high degree of monodispersity (5-6%) and a single-crystalline internal structure [4]. The particles have been deposited on a Si substrate to form highly ordered superstructures (mesocrystals) using a drop casting method. Structural characterization has been carried out using SEM, AFM, TEM and GISAXS. Depending on the shape of the particles, the arrays show mesostructures with bct [5] or fcc symmetry with relatively long structural correlation lengths of 2-10 μ m.

In order to investigate magnetic inter-particle correlations we have employed grazing incidence neutron scattering experiments in reflectometry mode at the JCNS-instrument TREFF at the FRM II in Garching and in GISANS mode at the Magnetism Reflectometer at the SNS in Oak Ridge and MARIA at FRM II in Garching. These experiments yielded the degree of magnetic correlation for the in-plane and out-of-plane directions at different applied fields.

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CT06

Diffusion Properties of metallic liquids and their binary alloys

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Liquid diffusion coefficients are key input parameters for modelling of solidification as well as important parameters for testing potentials used in molecular dynamics simulations. It has been shown that the simulated microstructure of a material sensitively depends on the diffusion coefficient [1]. Further it has been shown for a pure metal, Ti, that diffusion coefficients can be used to improve molecular dynamics simulations [2]. However, diffusion data for liquids are scarce compared with data available for solids and show typically a large error when obtained with conventional capillary experiments [3]. Consequently, the relation between self-, impurity and chemical diffusion in liquids, their temperature dependence, and their relation to thermophysical properties such as viscosity are still debated.

A comprehensive data set on self-, impurity, and chemical diffusion coefficients for pure metals, liquid Ge, and Al-based alloys is presented. Neutron time-of-flight spectroscopy was used to determine self diffusion coefficients with high accuracy whereas x-ray radiography in combination with capillary experiments was used to determine accurate impurity and interdiffusion coefficients in binary alloys. For liquid-Ge and liquid-Al it is shown that impurity diffusion coefficients do not depend on mass. For liquid-Ge a dependence of impurity diffusion on the covalent radius of the impurity atom is observed and impurity diffusion and solvent self-diffusion agree within error bars. At and around the melting point diffusivities are typically well described by an Arrhenius law. It is shown that the Stokes-Einstein relation predicts diffusivities based on viscosity data only within a factor two for pure liquid metals. Finally, measured interdiffusion coefficients for Al-Cu alloys are compared with calculated values using the empirical Darken relation and measured Cu self diffusion coefficients. These data are discussed in the context of recent findings by molecular dynamics simulations.

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CT07

Neutron scattering experiments on Zr-based melts processed by electrostatic levitation

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We have developed a compact electrostatic levitator as a sample environment for high quality neutron scattering experiments on melts [1]. This containerless technique allows to process even chemically reactive melts at high temperatures. Moreover, the containerless process under high vacuum conditions gives access to the metastable regime of an undercooled liquid below the melting temperature. The avoidance of crucible materials in the vicinity of the freely suspended sample results to an excellent signal to background ratio in scattering experiments.

The utilization of the electrostatic levitator allowed us to investigate the structure and the atomic dynamics of different stable and undercooled Zr-based melts by elastic- and quasielastic neutron scattering as a function of the temperature.

Quasielastic neutron scattering studies have been performed on the time-of-flight spectrometer TOFTOF at the FRM II. For liquid $\text{Zr}_{64}\text{Ni}_{36}$ the Ni self-diffusion coefficient shows deviations from an Arrhenius-type temperature dependence at an undercooling of 167 K below the melting point, as observed in also for bulk metallic glass forming alloys.

Elastic neutron diffraction experiments were performed on the high flux diffractometer D20 at the ILL. The structure factors measured for $\text{Zr}_{50}\text{Cu}_{50}$, $\text{Zr}_7\text{Cu}_{10}$ and Zr_2Cu revealed large nearest neighbor coordination numbers of $Z_{NN} > 13$. While it is widely assumed in literature that the good glass forming ability of Zr-Cu is related to an icosahedral short-range order prevailing in the melt, our investigations demonstrate that liquid Zr-Cu is not characterized by a dominant icosahedral short-range order.

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PT03

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CT08

Electron-phonon coupling in the conventional superconductor $\text{YNi}_2\text{B}_2\text{C}$ at high phonon energies studied by time-of-flight neutron spectroscopy

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We report an inelastic neutron scattering investigation of phonons with energies up to 159 meV in the conventional superconductor $\text{YNi}_2\text{B}_2\text{C}$. Using the SWEEP mode, a newly developed time-of-flight technique involving the continuous rotation of a single crystal specimen, allowed us to measure a four dimensional volume in (\mathbf{Q}, E) space and, thus, determine the properties of the A_{1g} (≈ 102 meV) and A_u (≈ 159 meV) type phonon modes. In particular, the A_{1g} mode, which modulates the bonding angle of the Ni-B tetrahedra, was predicted to have a decisive influence on superconductivity [1]. We used the high flux at large neutron energies available at the Spallation Neutron Source, Oak Ridge National Laboratory, combined with the SWEEP mode in order to map out the electron-phonon coupling of the high energy branches for the whole Brillouin zone. Despite of having linewidths of $\Gamma = 10$ meV, A_{1g} modes do not strongly contribute to the total electron-phonon coupling constant λ , i.e. less than 3 %. Nevertheless, contributions to λ stem dominantly from phonons with movements of the light B and C atoms but in modes with surprisingly low frequencies. We observe a remarkable agreement with *ab-initio* calculations over the complete phonon energy range demonstrating the accuracy of such calculations in a rare comparison to a comprehensive experimental data set.

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CT09

Chirality of the spin resonance in the unconventional superconductor CeCoIn₅ investigated with polarized neutrons under magnetic field

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In many unconventional (copper-oxide-, iron- or *f*-electron-based) superconductors a magnetic excitation is evidenced by inelastic neutron scattering (INS) below the superconducting transition temperature. This so-called spin resonance is visible at the wave-vector for which the superconducting gap, Δ , changes sign and for an energy $\Omega_{\text{res}}/2\Delta \approx 0.64$. While there is no consensus on the origin of such an excitation and its relevance for the pairing mechanism, it provides important information relative to the symmetry of the superconducting state and it allows thus to reveal the nature of this state.

It is therefore important to get more microscopic insight into the spin resonance and in particular to investigate the multiplicity of this excited state. The application of a magnetic field may lift its degeneracy and polarized neutron scattering technique is very powerful to analyse the corresponding fluctuations. Among unconventional superconductors, *f*-electron based compounds with their intrinsic low characteristic energy scales are particularly suitable to observe strong effects under magnetic field. Resonance peaks are reported so far for the heavy fermion systems UPd₂Al₃, CeCu₂Si₂ and CeCoIn₅.

Here we show by using polarized INS technique that the spin resonance in CeCoIn₅ splits under magnetic field and that the magnetic response is composed of three channels: two Zeeman split peaks that have a chiral nature and a supplementary non-chiral contribution appearing at the same energy than the lower mode of the Zeeman split peaks.

CT10

A neutron resonance spin-echo study of the symmetry of the order parameter in an iron-based superconductor

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The symmetry of the superconducting gap in the iron-based superconductors is still a matter of some debate in the literature. The observation of a neutron spin resonance by several groups [1] lends support to the s^{+-} order parameter picture [2], in which the sign of the superconducting gap changes between the electron and hole pockets of the Fermi surface. However it has been argued that a similar feature to the spin resonance could appear within the s^{++} description, where the sign of the gap does not change over the Fermi surface [3]. In our work we have implemented an alternative method to elucidate the order parameter symmetry [4]: by measuring the evolution of the energy and lifetime of phonons above and below the superconducting transition temperature T_c .

When a material passes into the superconducting state, the character of the electronic excitation spectrum is dramatically altered, which can impact upon phonon energies and phonon lifetimes. Below T_c the magnitude of the superconducting gap Δ increases with reducing temperature, so for phonons with sufficiently low energy E_{ph} there is a temperature T^* at which $2\Delta = E_{ph}$. For s -wave superconductors, the electronic density of states has a singularity at Δ , so at T^* one observes a large increase in the phonon linewidth, as the phonon can decay into two Bogoliubov quasiparticles of energy Δ . If the order parameter symmetry is more complicated, then the temperature evolution of the phonon linewidth is predicted to be strongly modified [4]. This phenomenon was recently studied in s -wave superconductors Pb and Nb using the neutron resonance spin-echo (NRSE) TRISP spectrometer, which is capable of resolving phonon linewidths in the μeV range [5] over the entire Brillouin zone.

Here we introduce the principles of the NRSE technique and present our measurements of phonon lifetimes in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ($x = 9\%$, $T_c = 24$ K). Despite our study being hampered by the lack of a low energy phonon (< 10 meV) at the Fermi surface nesting vector, we have found evidence for a possible departure from s^{+-} order parameter symmetry. We also communicate the observation of an anomaly in the phonon linewidth found perpendicular to the Fe-As planes, and discuss its unusual temperature dependence.

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CT11

Spin Fluctuations and Phonon Softening in the strongly correlated semiconductor FeSi

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FeSi is a narrow band gap semiconductor crystalizing in the cubic B20 structure missing an inversion center. Due to its unconventional electronic and magnetic properties which only have been observed in a class of heavy fermion systems known as Kondo insulators, it has often been claimed being the first 3d material belonging to this class of materials [1, 2]. More recently evidences for strong electron-phonon coupling have been observed by means of thermo transport measurements and inelastic neutron scattering experiments [3, 4]. Though bulk properties of FeSi were studied extensively, microscopic experimental information on spin fluctuations and the lattice dynamical properties of FeSi are scarce.

Here we report on detailed measurements on the magnetic excitation spectra and lattice dynamical properties using inelastic neutron scattering. Paramagnetic fluctuations have been investigated using polarized neutrons at the thermal triple axis spectrometer IN20, ILL, Grenoble down to temperature of 15K and up to energy transfers of 80 meV in order to search for the spin gap, which is supposed to be around 60 – 70 meV based on measurements of the temperature induced paramagnetism [5]. Our data show no evidence for any gapped spin fluctuations up to highest energy transfers. Even larger energy transfers up to 150 meV could be achieved at the chopper spectrometer ARCS, SNS [6]. Still, no temperature-induced changes, which might indicate a redistribution of spectral weight, were observed for $E \geq 70$ meV between $T = 15$ K and 300 K.

Further we measured the low temperature phonon dispersion along the main crystallographic directions over the complete frequency range ($E \leq 60$ meV) by means of inelastic neutron scattering. The experimental results are compared with theoretical calculations based on DFT within the LDA approximation. Certain phonon branches have been investigated in more detail with regard to the temperature dependence in a temperature range from 10K – 800K. In order to distinguish between normal and anomalous softening of the phonon spectra, results are compared to calculations using lattice constants corresponding to different temperatures.

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PT04

Structure of soft lyotropic crystals and quasicrystals

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Micelles are the most abundant example of self-assembly. In aqueous solutions micelles can form highly ordered lyotropic liquid crystalline phases. Using shear orientation it is possible to obtain highly ordered single crystalline samples showing more than 100 Bragg reflections. With scanning small-angle neutron diffraction it is possible to map the complete reciprocal space and analyse the structure of such soft crystals in great detail. With this method we could not only characterize structures exhibiting classical crystallographic order, but also newly discovered lyotropic quasicrystals with 12- and 18-fold rotational symmetry.

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CT12

The motions in liquid *n*-alkanes: A neutron scattering and MD simulations study

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The self-diffusion in molecular liquids is a result of several local motions of the molecules. These motions can be pictured as e.g. tumbling of methylene groups or global rotation of the entire molecules. The understanding of these processes and their interactions is essential for the description of the transport mechanism in molecular systems.

In order to probe these basic dynamics in the pico- to nanosecond time regime and on a molecular length scale, resolution resolved time-of-flight quasi-elastic neutron scattering (TOF-QENS) experiments were performed on various short- and medium-chain *n*-alkanes. It was found that the dominating relaxation processes obey a Q^2 -dependence of the broadening of the elastic line, indicating a Fickian diffusion behaviour [1]. However, a comparison of the apparent diffusion coefficient with the long-time long-range values determined by pulsed-field-gradient nuclear magnetic resonance (PFG-NMR) shows that the observed motions cannot be attributed to centre-of-mass long-range diffusion [2].

Neutron scattering experiments alone cannot identify these prevailing motions. Therefore detailed molecular dynamics (MD) simulations were performed, which represent the measured data nicely [3]. A comparison of the QENS data with the MD simulations shows that the dynamics in the QENS time window mainly arise from local bond rotations, leading to a reorientation of the entire molecules. With increasing chain length these global dynamics emerge from the picosecond time window, whereas more complex intramolecular dynamics appear.

With this powerful combination of QENS experiments and MD simulations we are able to present a detailed picture of the diffusional processes in the whole picosecond time regime.

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CT13

Phase Separation and Molecular Intermixing in Polymer-Fullerene Bulk Heterojunction Thin Films

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The performance of solution processible organic photovoltaic devices improved continuously during the last years. Over the recent years continuous progress was made concerning the efficiency of polymer solar cells reaching meanwhile values above 10%.¹ Major improvements were achieved with the bulk heterojunction concept^{2,3}, due to the increased inner acceptor-donor interface, and with the development of new semi-conducting small band-gap polymers. However, despite the increase in efficiencies, deep fundamental understanding is still limited.

In the last years the blend out of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61 butyric acid methyl ester (PCBM) established as the best investigated system in organic photovoltaic devices.⁴ While these investigations addressed mainly domain structures or the diffusion and the miscibility of PCBM in the P3HT phase, we focus in the presented work on the detailed structure, i.e. phase sizes, structural length scales, and molecular miscibility of the components, in a P3HT:PCBM bulk heterojunction. Grazing incidence small angle neutron scattering (GISANS) combined with a detailed analysis is used to extract structural information as well as molecular mixing of P3HT and PCBM films.⁵ The analysis is based on the distorted wave Born approximation (DWBA) as shown in figure 1.

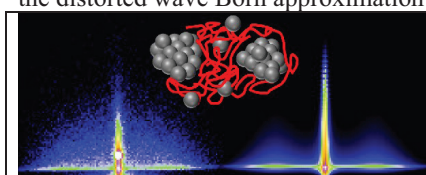


Fig. 1: 2d GISANS data (left) and corresponding 2d simulations (right) of P3HT:PCBM BHJ film with 33wt% PCBM. Inset shows the model used in the simulation. Taken from reference [5].

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CT14

Dynamics and Structure of Polyelectrolytes in Aggregates with Oppositely Charged Surfactants

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Systems composed of oppositely charged polyelectrolytes and surfactants show rich self-aggregation behavior that varies over a large size range and have many applications e.g. in cosmetics, detergency and drug delivery. Mixtures of the cationic polyelectrolyte JR 400 with anionic surfactants (SDS, SDBS) in the semi-dilute regime with a slight excess of polymer charges form highly viscous network structures, with their viscosity increasing by 3-4 orders of magnitude as compared with the pure polymer solution, while mixtures with excess surfactant charges form solutions with viscosities even below those of the polymer solution[1,2]. In this study we investigated the structure of the polyelectrolyte chain in the aggregates with the aid of small-angle neutron scattering (SANS).

Furthermore, the dynamics of the polyelectrolyte has been studied with the help of Neutron Spin-Echo (NSE). Previous studies with Dynamic Light Scattering (DLS) have shown, that data can be described in terms of the mode-coupling theory. However, NSE allows to access significantly smaller size ranges, corresponding to the aggregates seen in SANS. Therefore the dynamics of local segments of individual chains and of the micellar aggregates are monitored rather than those of larger clusters as in DLS. Measurements show that the effect on the dynamics is much less pronounced in NSE as compared to DLS.

In summary, we studied the behaviour of polyelectrolytes in solutions of mixed aggregates of polyelectrolytes and oppositely charged surfactants with the help of neutron scattering, gaining an understanding of the role that the polyelectrolyte component plays in the formation of such aggregates and in particular with respect to its dynamic properties. This understanding can be valuable for the design of future formulations.

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CT15

Ring Rotation Dynamics of Ferrocene and Ferrocene-containing Polymers

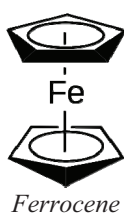
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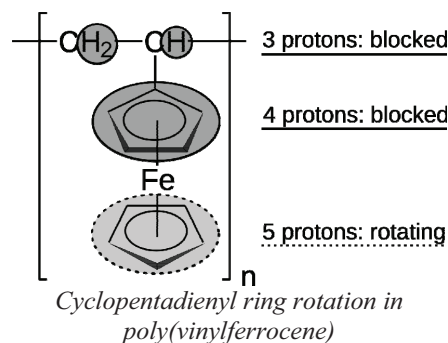


Ferrocene is an organometallic compound consisting of two cyclopentadienyl rings with a reversibly oxidizable iron atom sandwiched in between (see left). Bulk ferrocene shows a structural phase transition at 164K (triclinic to monoclinic). Ferrocene-containing polymers are of interest for applications in nanotechnology as they combine polymeric with metallic properties and can show ferromagnetic susceptibilities [1]. As an important aspect of the characterization of ferrocene-containing polymers we study the cyclo-pentadienyl ring rotation dynamics. We aim

to compare the ring rotation of bulk ferrocene to ferrocene contained in polymers using inelastic neutron scattering.

In bulk ferrocene, past neutron scattering studies of the ring rotation dynamics mainly focussed on the high temperature phase [2]. We refine and extend the results to the low temperature phase using neutron time-of-flight and backscattering experiments including the new possibility of inelastic fixed window scans (IFWS) on IN16 at the ILL [3]. The extracted correlation times and activation energy of the rotation dynamics are found to be considerably higher than for the high temperature phase.

In poly(vinylferrocene), the ferrocene complex is laterally attached to a polymer chain. Additionally to time-of-flight spectroscopy we use polarized neutron diffraction to separate coherent from incoherent scattering in order to measure the static structure factor of the amorphous polymer. The combination of diffraction and spectroscopy enables us to extract the elastic incoherent structure factor (EISF). The resulting EISF supports the assumption that only one ring of the ferrocene sandwich complex is rotating according to a 5-fold circular jump diffusion model (see figure).



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PT05

Precision measurements with cold neutrons

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Precision measurements of properties of the neutron or its decay yield important parameters of the standard model of particle physics but are also used to search for new particles or interactions. These experiments are complementary to high-energy physics at colliders. Their requirements, for example in terms of neutron polarisation or intensity, push developments of neutron techniques. I will review recent experiments with cold neutrons and discuss technological challenges and achievements.

CT16

Dynamics of microemulsions adjacent to planar hydrophilic walls

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Aqueous surfactant systems have manifold applications for the enhanced oil recovery. The micelle formation of the surfactant leads to high viscosities, which is desired for many reasons. The cracking fluid needs to deposit the hydrostatic energy in the sand stone close to the bore hole, and, thus, cracks are generated. The proppant consists of sand particles, which are left inside the cracks and keep the porosity high for better production rates after the application. The fluid itself forms a microemulsion when in contact with oil. The microemulsion possesses a low viscosity, which is favorable for the easy production.

The static structure of a bicontinuous microemulsion as a model complex fluid has been studied statically by GISANS and reflectometry experiments and in parallel by computer simulations [1]. A lamellar structure was induced by the planar wall. The high order decayed with growing distance from the wall and finally the bulk structure is bicontinuous. The decay of the lamellar order was realized by a growing number of perforations as observed by the simulations. The typical lengths of the decay and the onset of the perforations were compared between the different methods.

Dynamically, the grazing incidence method was transferred to neutron spin echo spectroscopy [2]. We found three times faster relaxations close to the wall in comparison to the bulk structure. The hydrodynamic waves are reflected by the wall, which explains the faster undulations of the surface near lamellae. Faster dynamics explain also a lower viscosity, which in this case is known as the lubrication effect. This effect would theoretically explain a slip length indicating a facilitated sliding off of the oriented lamellae. This in turn is highly interesting for flow fields of complex fluids in porous materials or for an initial state in the capture process of immune cells at vessel walls.

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CT17

Quantum mechanical effects in superconductors visualized and quantified with polarized neutrons

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The most prominent macroscopic quantum mechanical effects in superconductivity are the well known zero electrical resistance and the Meissner effect (magnetic field expulsion), less known is the effect of magnetic flux trapping (pinning) in materials in their superconducting intermediate state. The investigations of flux trapping are still subject of many publications since L. Landau proposed in 1938 a solution that a body in the intermediate state consists of alternating layers of superconducting and normal phase [1]. The intermediate state reveals phenomena that were not predicted by the first theories, and experiments are still necessary to understand better flux trapping/pinning in type-I superconductors [2]-[4].

Recent investigations with the new instrument for polarized neutron tomography (PONTO) with large ($> \text{cm}^3$) and virtually zero demagnetization samples (lead, superconductor type-I and niobium, type-II) yielded very surprising results [5], [6]. It could be shown that both the Meissner effect and flux trapping in high purity lead samples (type-I superconductor) occur different for the crystalline (mosaic spread 1.7°) and extreme homogeneous and pure (99.999wt-%) polycrystalline samples, respectively.

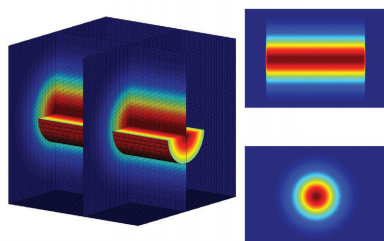


Fig.1 Shape of the calculated trapped magnetic field

The trapped flux of an uniform external magnetic field applied to the lead polycrystalline samples is for $T < T_c$ not uniform distributed but centered and squeezed around the rod axis of the samples (see Fig.1). Calculations concerning the partial Meissner effect and flux trapping agree perfectly with experimental resulting images if a "squeezed" Gaussian shaped B-field is assumed.

This work was part of BMBF project 05K10KF1.

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PT06

Scientific Strategy for the European Spallation Source

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The European Spallation Source (ESS) is a joint project sponsored by 17 European countries, to build the worlds brightest neutron source for the study of materials and fundamental physics. ESS aims to accelerate protons up to 2 GeV and 50 mA to generate neutrons using spallation from a rotating heavy element target. The neutron pulses that ESS will generate will be more that 30 times brighter than the world's brightest reactor based sources. In the ESS pre-construction phase, the European neutron community are participating in an extensive instrument conceptual design effort, as well as in workshops and symposia to discuss the best way to utilize the scientific opportunities that ESS will offer. In this talk, I will outline the scientific drivers and strategy of ESS and how these are manifested in the suite of instruments that is currently under development.

PT07

The German contribution to the ESS Design Update Phase

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In 2019, the European Spallation Source (ESS), a joint project of 17 European countries, is planning to start operation, initially with 7 instruments. It will be the most powerful neutron source in the world and will facilitate unique insights into matter both for basic research and application-oriented research. The construction start is planned for 2013, and plans call for the number of instruments to be increased to 22 by 2025.

The Federal Ministry of Education and Research (BMBF) has provided funding for the contribution of Germany to the design-update phase of the ESS. Seven research centres in Germany participate in this collaborative project which runs from 2010 to 2013. In 22 workpackages design work on the accelerator, target and instrumentation is done giving Germany a pioneering role among the European partner countries. Furthermore, the evaluation of scientific opportunities and requirements of the German neutron users is an integral part of the project, allowing the neutron community to take part in the design and construction of the ESS and its science.

The work and activities within the German collaborative ESS design update project are presented.

PT08

Spectroscopy of Gravity

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Cosmological parameters describe the properties and the global dynamics of the universe. Observational cosmology has determined these parameters to one or two significant figure accuracy. Of great interest is now how the energy-matter budget is built up from its constituents: baryons, photons, neutrinos, dark matter and dark energy. The known particles of the Standard Model account for only 4%, whereas the majority consists of unknown dark energy and dark matter.

Both dark energy and dark matter might show up as tiny signals in gravity experiments and disclose their identity as e.g. a chameleon particle or an axion particle. They have triggered research of different kinds, which in the past ten years have validated Newton's gravitational law down to about 50 μm .

Missing so far were experiments with an absolute energy calibration based on natural constants and elementary particles. We present here a frequency ladder with a spacing based on the speed of light c , the Planck constant h , the mass of the neutron m_n , and the acceleration of the earth g in the quantized gravity potential of the earth, which is probed by a resonant spectroscopy technique.

In contrast to the frequency comb in laser spectroscopy, the frequencies in the gravity potential are not equidistant but given by the Airy-Functions, which allows us to use a resonant spectroscopy technique to probe the energies. A measurement of several discrete energy eigenstates of a neutron in the gravity potential of the earth in comparison with Newton's gravity law sets exclusion limits on the pseudoscalar axion-coupling in the previously inaccessible astrophysical axion-window or to scalar fields (chamelions).

PT09

Neutrons and Energy materials: Present research and future opportunities

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Achieving sustainability in the energy economy is a major declared societal goal of the European union and most notably of the German government. As in a very large part, energy relevant problems are ultimately materials problem, neutron scattering and its unique ability to shed a penetrating light at the microscopic scale into the materials structure, kinetics, and dynamics is a relevant and important technique. Many type of energy materials, from hydrogen storage materials to thermoelectrics can be successfully investigated with neutron scattering techniques. However, the complexity and rather difficult data analysis is a major hurdle in involving a broader community of materials scientists working directly on energy problems. In this overview, after setting the stage of the energy landscape of today and the targets for tomorrow, selected examples of problems in which neutrons have provided important insights will be presented. The major insights gained in the framework of 'Neutrons for global energy solutions' will be summarized and possibly opportunities for future research at existing and new neutrons sources will be discussed.

PT10

Providing insight on bio-molecular interactions with biological membranes by using neutron scattering techniques - challenges and outlook

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The biological membrane is one of the most important interfaces that the drug delivery vehicles encounter. The barrier function of the membrane is provided by the lipid bilayer. Lipids and lipid self-assembly structures are important as regulators for biological activity that can be exploited for the design of drug delivery vehicles. One important aspect is how these vehicles interact with different artificial as well as biointerfaces including biological membranes. Simple supported lipid bilayers as models for biological membranes have allowed us to study the biophysics of biomolecular interactions using neutron reflectometry as well as a range of other surface techniques. Based on our results we will discuss how such studies could be extended to more realistic models.

Modern medicine has found ways to treat diseases, caused by genetic defects, by “repairing” the DNA, so-called gene therapy. One of the main challenges with gene therapy is to deliver the nucleic acids across the membrane. Knowledge of how DNA and RNA interact with lipids is central to the understanding of organization and function of these molecules in biological systems. The main obstacle here is the charge as well as the extensive size of the DNA in solution. In gene therapy one often utilizes vehicles with the ability to condense DNA and thereby protect DNA against degradation, transport DNA across membranes as well as regulate gene expression. The compacting agent not only condenses the DNA chain, but depending on the nature and the strength of the interaction often can form intriguing morphologies. We will discuss how neutrons could extend the knowledge of the DNA and RNA interaction with the lipid membrane. This will give new knowledge of the nature of this interaction and how it can be manipulated with compacting agents.

PT11

Emergent Phenomena of Complex Electronic Materials

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Complex electronic materials display emergent phenomena in intimate analogy with a wide range of different areas in physics. Examples include the Higgs mechanism in superconductors, magnetic monopoles in frustrated magnets and Majorana fermions in topological insulators. I will present recent experimental studies in chiral magnets that allude to a research program initiated by Heisenberg, notably how to go beyond particle-wave duality. Using neutron scattering we identified a new form of magnetic order in certain chiral magnets, which is composed of topologically stable knots in the spin structure, so-called skyrmions. The skyrmions may be viewed as particle-like states of continuous fields, forming lattice structures as well as amorphous and glassy phases reminiscent of vortex lines in superconductors. In the electronic transport properties the skyrmions give rise to a quantized Berry phase causing a new form of Hall effect, the topological Hall effect. Most remarkably, perhaps, we observe large spin transfer torques mediated by this Berry phase at ultra-low current densities. This illustrates how emergent phenomena of complex electronic materials connect issues across a wide range of areas in physics with challenges in applied physics.

PT12

„Wolfram-Prandl Prize Lecture“

NN

Der mit 2500 Euro dotierte Wolfram-Prandl-Preis wird vom KFN während der diesjährigen Deutschen Neutronenstreutagung für eine hervorragende Arbeit, bei der Untersuchungen mit Neutronen einen wesentlichen Anteil hatten, an eine/n Nachwuchswissenschaftler/in vergeben. Dabei sollen Methodenentwicklung und Fundamental Physics ausdrücklich in die Betrachtung einbezogen werden.

Talks Wednesday, September 26, 2012

- PT13 B. Nickel
Asymmetry and phase separation in lipid membranes
- CT18 F. Schreiber
Phase behaviour and associated dynamics of protein solutions manipulated by ions
- CT19 T. Nawroth
Bio-nanoparticles for medical applications, enhancer radiotherapy - SANS, DLS & ASAXS
- CT20 A. Stadler
Thermal fluctuations of haemoglobin from different species: Adaptation to temperature via conformational dynamics
- CT21 M. Schmiele
Small angle scattering study on the stabilizer layer in triglyceride suspensions
- PT14 M. Angst
Multiferroicity from charge ordering? A case study
- CT22 D. Lott
Chirality effects in rare-earth multilayers investigated by polarized neutrons
- CT23 O. Petravic
Magnetic correlations in dipolarly coupled iron oxide monolayer and multilayer films
- CT24 V. Zhernenkov
RF field stimulated magnetization kinetics probed in thin films with MIEZE based Time-Resolved AC (TRAC) PNR
- CT25 M. Loewenhaupt
Low-energy and crystal field excitations in single-crystalline CeCu_2Ge_2 in fields up to 12 T
- CT26 F. Groitl
Larmor labeling methods: Neutron resonance spin echo spectroscopy beyond standard line width measurements
- CT27 A. Radulescu
KWS-2 – the high-intensity / wide Q-range small-angle neutron diffractometer with tunable resolution at the FRM II optimized for soft-matter and biology
- CT28 P. Lindner
Recent developments in sample environment for SANS at D11@ILL
- CT29 E. Babcock
Polarization analysis with ^3He spin filters to separate coherent scattering from total scattering in SANS
- CT30 W. Kreuzpaintner
In-situ neutron reflectometry during thin film growth by sputter deposition
- CT31 F. Mezei
Neutron generation and beam extraction at ESS

PT13

Asymmetry and phase separation in lipid membranes

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Lipid bilayers with controlled content of anionic lipids are a prerequisite for the quantitative study of hydrophobic-electrostatic interactions of proteins with lipid bilayers. Here, the asymmetric distribution of zwitterionic and anionic lipids in supported lipid bilayers is studied by neutron reflectometry at REFSANS. NR reveals the presence of anionic lipids (d₃₁-POPS) in the outer bilayer leaflet only, while no POPS is observed in the leaflet facing the SiO₂ substrate [1]. We argue that this asymmetric distribution of POPS is induced by electrostatic repulsion of the phosphatidylserines from the negatively charged hydroxy-surface groups of the silicon block. Such bilayers with controlled and high content of anionic lipids in the outer leaflet are versatile platforms to study anionic lipid protein interactions which are key elements in signal transduction pathways at the cytoplasmic leaflet of eukaryotic cells. Furthermore, we report GISANS experiments to study phase separation in mixed bilayers.

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CT18

Phase Behaviour and Associated Dynamics of Protein Solutions Manipulated by Ions

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We will discuss how mono- and multivalent ions can be used to manipulate the interactions and the associated phase behaviour as well as the associated diffusion dynamics of aqueous protein solutions. In particular, we show that multivalent ions do not only influence the ionic strength and the effective interactions in aqueous solutions [1], but lead to qualitatively new effects. Specific attention will be given to the "reentrant condensation" of proteins [2,3] and its relationship with liquid-liquid phase separation and crystallization. In this context, we attempt to rationalize crystallization controlled by trivalent ions [4,5].

We will first focus on results obtained by elastic scattering, in particular SANS using contrast variation in comparison with SAXS and ASAXS, extracting information on the ionic and water shell around the proteins (based on the form factor) as well as the interactions (based on the structure factor) [6].

Second, we will discuss the consequences on the dynamics of these systems for different salt concentrations (i.e. with different effective interactions), different crowding conditions (protein concentration) and also near salt-induced phase transitions. This involves both quasi-elastic neutron scattering (QENS) [7] as well as dynamic light scattering techniques (DLS) [8].

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CT19

Bio-Nanoparticles for Medical Applications, Enhancer Radiotherapy - SANS, DLS & ASAXS

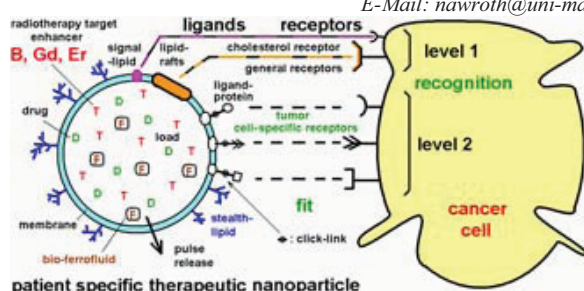
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Concept of Tumor-case specific target nanoparticles, liposomes with **two levels** of ligands: 1.) lipids and rafts generate moderate attraction; 2.) for **case specific recognition receptor** ligands at level 2 are bound as a mix (~3) by cleavable links with a fast click-chemistry (e.g. S-S linked ligands)

patient specific therapeutic nanoparticle

Target Nanoparticles can enforce radio- and chemotherapy of cancer in two ways: concentration of the drug in particles, and targeted localization of therapeutic material in the tumor. A further advantage is the case-selective uptake and delivery at cellular level by endocytosis. For radiotherapy the drug is an enhancer, which enforces the radiation induced cell inactivation by the high absorption cross section of heavy elements or special isotopes.

Our therapeutic nanoparticles for enhanced radiotherapy are combined from lipids, bio-polymers and magnetic iron oxides in a modular system. The particles of ~100 nm size carry an enhancer load of lanthanide complexes or boron as radiation absorption target and proliferation inhibitors. A major object are target liposomes bearing modular surface signals for cell recognition, and the drug, e.g. lanthanides (Gd, Er, Lu). A premature degradation of the therapeutic target nanoparticles is avoided by novel stealth lipids bearing a polyglycerol head [1]. Other nanoparticles bear polymers and bio-ferrofluids for magnetic manipulation, MDT [2].

The particles are characterized [3] by dynamic light scattering DLS, electron microscopy, neutron scattering SANS, anomalous X-ray scattering ASAXS, X-ray-imaging, and magnetic characterization. The biocompatibility and therapeutic effect is investigated with cancer cell cultures of several lines of brain, lung, liver, colon and kidney cancer. In our kinetic EPN test cell cultures are used as 2D tumor models. This distinguishes between a radio-toxic action and the favored cancer cell proliferation inhibition, which is equivalent to a tumor growth stop. This can be done as high-throughput test with MTT [4]. As radiation sources for therapy tests we use for neutron capture therapy NCT the reactors TRIGA Mainz (thermal), and ILL Grenoble (cold neutrons), for photon therapy the linear accelerators at the radiooncology clinics Mainz (8 MeV), and for monochromatic radiation of ~60 keV the ESRF synchrotron.

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CT20

Thermal Fluctuations of Haemoglobin from Different Species: Adaptation to Temperature via Conformational Dynamics

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Thermodynamic stability, configurational motions, and internal forces of haemoglobin (Hb) of three endotherms (platypus - *Ornithorhynchus anatinus*, domestic chicken - *Gallus gallus domesticus* and human - *Homo sapiens*) and an ectotherm (salt water crocodile - *Crocodylus porosus*) were investigated using circular dichroism, incoherent elastic neutron scattering, and coarse-grained Brownian dynamics simulations. The experimental results from Hb solutions revealed a direct correlation between protein resilience, melting temperature and average body temperature of the different species on the 0.1 ns time scale. Molecular forces appeared to be adapted to permit conformational fluctuations with a root mean square displacement close to 1.2 Å at the corresponding average body temperature of the endotherms. Strong forces within crocodile Hb maintain the amplitudes of motion within a narrow limit over the entire temperature range in which the animal lives. In fully hydrated powder samples of human and chicken Hb mean square displacements and effective force constants on the 1 ns time scale showed no differences over the whole temperature range from 10 to 300 K, in contrast to the solution case. A complementary result of the study, therefore, is that one hydration layer is not sufficient to activate all conformational fluctuations of Hb in the pico- to nanosecond time scale which might be relevant for biological function. Coarse-grained Brownian dynamics simulations permitted to explore residue specific effects. They indicated that temperature sensing of human and chicken Hb occurs mainly at residues lining internal cavities in the β subunits.

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CT21

Small angle scattering study on the stabilizer layer in triglyceride suspensions

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Suspensions of triglyceride solid lipid nanoparticles are studied in modern pharmaceutical research as a potential drug delivery system [1] and are also of peculiar interest in food science. Our research group focuses on dispersions of tripalmitin nanocrystals that are stabilized by well-tolerated phospholipids and bile salts in an aqueous dispersion medium. These dispersions can be considered as a representative model for many similar colloidal dispersions intended for drug delivery. Revealing the molecular arrangement of the amphiphilic phospholipid molecules at the interface between the lipid tripalmitin core and the aqueous phase is crucial to understand the nanoparticle's stabilization mechanism but also to control their drug encapsulation ability. However, up to today the knowledge about the structural arrangement of the phospholipid molecules in the stabilizer layer is rather vague. Do the lipophilic acyl chains of the phospholipids stick into the tripalmitin core or are the complete molecules just sitting on top of the tripalmitin matrix ? On average, is the stabilizer layer a monolayer or a multilayer ? Combining small angle x-ray and neutron scattering data and utilizing the contrast variation technique our group tries to find a more meaningful model for the phospholipid stabilizer layer.

Tripalmitin and many other organic substances possess long crystallographic c-axes and as a result exhibit Bragg peaks in the small angle scattering range. Interestingly, in a previous SAXS study it turned out that tripalmitin's 001-Bragg reflection is very sensitive on the stabilizer layer properties (thickness and scattering contrast) what can be utilized to resolve their structure [2]. For the simulation of small angle scattering patterns of dispersions of homogeneous nanoparticles a plenty of software packages do exist and they, basically, all rely on the calculation of the particle form factor. However, by this approach the existing simulation programs can take Bragg reflections into account only by heuristic models for their peak profiles. To remedy this shortcoming and to compute small angle scattering patterns from colloidal dispersions of crystalline nanoparticles the "X-Ray Powder Pattern Simulation Analysis" (XPPSA) method has been developed [2] and extended for neutron scattering. It directly facilitates the computation of not only the small angle scattering but also of the Bragg scattering contributions from a statistical particle model and the geometry of the nanocrystals and their stabilizer layer.

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PT14

Multiferroicity from charge ordering? A case study

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Magnetoelectric multiferroics have a large applications potential and often involve complex phase competitions. Among different possible mechanisms of multiferroicity, ferroelectricity originating from charge ordering is particularly intriguing because it potentially combines large electric polarizations with strong magnetoelectric couplings – but example materials where this is realized seem to be very difficult to find. After LuFe_2O_4 had been proposed to be a multiferroic due to ferroelectricity originating from $\text{Fe}^{2+}/\text{Fe}^{3+}$ charge order in 2005 [1], this material has become the generally accepted prototypical example of this mechanism and has correspondingly attracted increasing attention. The proposal had been made due to indications of a polar state by dielectric and pyroelectric measurements, and a reasonable model of charge order based on the location of superstructure reflections by X-ray diffraction. This charge order model has not been completely verified though [2], and the spin-order has also been a largely open question. I will present recent x-ray and neutron diffraction, and circular dichroism, measurements that now allowed i) a full refinement of the charge-ordered crystal structure [3], ii) the determination of the spin structures in two competing magnetic phases that are nearly degenerate at $T_N=240$ K [4], and iii) the relation between these orderings [3]. The results reveal a very strong coupling between spin- and charge order even in the precursor region to 3D long-range order, but also strong oxygen-stoichiometry dependences of all properties. Most importantly, the unambiguously determined arrangement of Fe^{2+} and Fe^{3+} ions excludes any charger-order-based ferroelectricity, implying that a clear example material for this mechanism has yet to be identified. I will also briefly discuss very recent dielectric spectroscopy results [5] that attribute the original macroscopic indications of ferroelectricity to artifacts, consistent with the microscopic findings.

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CT22

Chirality effects in Rare-Earth Multilayers investigated by polarized neutrons

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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 attention 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 reflectometry 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. 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.

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CT23

Magnetic correlations in dipolarly coupled iron oxide monolayer and multilayer films

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Self-assembled magnetic nanoparticles (NPs) have promising applications in future electronic and magnetic nano-devices [1]. The collective properties of self-assembled NPs strongly differ from those of the individual building blocks. This is due to the structural and magnetic ordering inside self-assembled systems. Particularly magnetic dipolar coupling can suppress thermal fluctuations and can lead to long-range ordering of the NPs. Polarized neutron reflectivity (PNR) provides a unique method to investigate both the structural and magnetic ordering [2]. We prepared iron oxide NP (diameter = 20 ± 1.4 nm) monolayer and multilayer films on a silicon substrate by spin-coating method. The NPs are arranged in a hexagonal close-packed geometry. Annealing at 230° C in vacuum yields magnetite (Fe_3O_4) as the major phase as confirmed from x-ray diffraction and magnetometry measurements [3]. PNR measurements were performed using the Super ADAM reflectometer stationed at ILL, Grenoble. In case of the multilayer the PNR shows a multilayer Bragg peak indicating a high degree of out-of-plane ordering. The magnetic correlation was deduced from the fitting of the PNR curves. In addition, the magnetic correlation in a monolayer was deduced in a special approach, where neutron standing waves were formed by creating a neutron potential well. The well consists of a vanadium film (50 nm) sandwiched between iron oxide NPs and an Al_2O_3 substrate. In remanence, the NP films (both monolayer and multilayer) show that dipolar coupling among the NPs lead to formation of quasi-domains resembling a superferromagnet [4].

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CT24

RF field stimulated magnetization kinetics probed in thin films with MIEZE based Time-Resolved AC (TRAC) PNR

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Since many decades the response of magnetization to static magnetic fields was thoroughly studied in different systems, e.g. thin continuous and laterally patterned films and multilayers, applying various experimental techniques [1]. However, in the recent years much attention is paid to the study of dynamic processes under the influence of alternating magnetic fields. One of the important tasks is the determination of the re-magnetization regimes and the role of e.g. different terms in the Landau-Lifshits-Gilbert (LLG) equation over a broad frequency range. This task can be approached with Time-Resolved AC (TRAC) Polarized Neutron Reflectometry (PNR) which records a time evolution of the depth resolved magnetization profile in the sample subjected to AC field. Due to uncertainties in the neutron flight-path, wavelength spread, etc. this “brut force” method applies at relatively low AC frequencies. However, the time modulation of the incident beam provided with the MIEZE setup solves the problem and substantially increases the applicability range of TRAC PNR. The latter gives a unique access to the frequency dispersion of longitudinal and transverse components of the retarded non-linear response function of the system. The experimental data were collected from thin Fe film placed in crossed DC and AC magnetic fields in a 40 – 350 kHz frequency range. It is shown that at low frequencies the net magnetization adiabatically follows the AC field. At higher frequencies, however, the retardation effect starts to play a role.

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CT25

Low-energy and crystal field excitations in single-crystalline CeCu_2Ge_2 in fields up to 12 T

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CeCu_2Ge_2 is a magnetically ordered ($T_N = 4.1$ K) Kondo lattice with a moderate enhanced Sommerfeld coefficient of 140 mJ/molK^2 . We performed inelastic neutron scattering experiments on a 2 g single crystal of CeCu_2Ge_2 using the cold triple-axis spectrometer PANDA at FRM II covering the low-energy “magnon”-range below 2 meV up to the crystal field excitations at around 18 meV [1]. Data were taken between 0.5 K and 10 K and in magnetic fields up to 12 T applied perpendicular to the (110/001) scattering plane. At zero field the low-energy magnetic excitations show an energy gap of 0.5 meV at all investigated Gamma points in the (110/001) plane with similar intensities. Away from the Gamma points the magnetic excitations become dispersive merging into a band of excitations around 1 meV. For increasing magnetic fields the gap energy decreases indicating opposite action of external and internal magnetic fields. Concomitant the crystal field excitations broaden and decrease slightly in average energy. The results will be discussed in the framework of local, crystal field related, and non-local, spin-wave-like, magnetic excitations. The possibility of a quantum phase transition at 8 T [2] is also discussed.

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CT26

Larmor labeling methods: Neutron Resonance Spin Echo spectroscopy beyond standard line width measurements

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We explore new territory for Neutron Resonance Spin Echo (NRSE) spectroscopy beyond measuring lifetimes of elementary excitations and present two experiments which benefit from the high resolution offered by this method. The first experiment aims at separating modes split in energy which are difficult to resolve with standard neutron scattering techniques [1]. In this context it is essential to take violation of the spin echo conditions and arbitrary local gradients of the dispersion surface into account which we provide with an extended model of the NRSE resolution function [2]. The second class of experiments deals with line shape analysis relevant for the phenomenon of asymmetric line broadening [3]. Measurements were performed on $\text{Cu}(\text{NO}_3)_2 \cdot 2,5\text{D}_2\text{O}$, a model material for a 1-D bond alternating Heisenberg chain, and on $\text{Sr}_3\text{Cr}_2\text{O}_8$, a dimerized spin-1/2 antiferromagnet. This is the first time this effect has been measured with high-resolution NRSE. The particular advantage of the NRSE method is the direct access to the line shape since there is no convolution of the signal with the resolution function of the spectrometer. Our experimental results show clear evidence for double peaked line shapes rather than a continuous asymmetry.

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CT27

KWS-2 – the high-intensity / wide Q-range small-angle neutron diffractometer with tunable resolution at the FRM II optimized for soft-matter and biology

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KWS-2 is a classical pinhole SANS diffractometer where the exploration of wide momentum transfers Q , from 6×10^{-4} to 0.5 \AA^{-1} , is possible by the variation of the sample-to-detector distance between 1m and 20m and of the wavelength between 4.5 \AA and 20 \AA . The instrument was recently upgraded and optimized towards high-intensity/extended Q -range investigations with tunable resolution of mesoscopic structures and structural changes due to rapid kinetics in soft-matter and biology. The high-intensity mode is sustained by (i) the high flux supplied by the cold neutron source of FRM II, (ii) the high efficiency ($>95\%$ for $\lambda > 4.5 \text{ \AA}$) ^6Li -scintillation detector, (iii) the fast detection electronics enabling high counting rates up to 0.6MHz, (iv) the high-intensity dedicated velocity selector ($\Delta\lambda/\lambda=20\%$), (v) the upgraded collimation system allowing for a routine use of large beam-size and (vi) the focusing elements – MgF_2 aspherical lenses – allowing for intensity gain compared to the conventional pinhole mode for the same resolution, due to increasing of the sample size (up to 5cm in diameter). With these opportunities the study of rapid kinetic processes within the sub-second range became a routine option. A double-disc chopper enables the tuning of the resolution and an improved characterization of the scattering features within different Q ranges using the time-of-flight method. The available Q -range can be extended towards low Q (up to $1.0 \times 10^{-4} \text{ \AA}^{-1}$) by means of MgF_2 lenses, which used in combination with the chopper (minimizing the chromatic aberrations and gravity effects) and a high resolution (0.5mm) position-sensitive detector, enable exploration of sizes up to 1 micron in a direct easy-to-handle fashion. With all these upgrades allowing for the boosting of its performance KWS-2 will be routinely operational in complete multi-functional configuration – standard pinhole, extended Q -range, high-intensity and tunable-resolution modes – by the end of 2012.

Near future upgrades will concern the improvement of the instrument performance for the exploration of short length scales typical for biological and semicrystalline systems. The extension of the Q -range towards 1 \AA is foreseen by aiming to shorter wavelengths (down to $\lambda=3 \text{ \AA}$) achievable by tilting the velocity selector. Additionally, the unambiguous acquisition of weak coherent signals from small and / or highly diluted structures fully corrected of incoherent scattering background that typically prevails at high Q will be possible after the installation of a transmission polarizer which will be used in combination with a wide-angle ^3He spin analyzing cell. The instrument options and performance will be reported.

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Recent developments in sample environment for SANS at D11@ILL

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D11 is one of the three SANS instruments at the ILL. All three SANS instruments (D11, D22 and D33) are designed to be versatile. Nevertheless, particular strengths of the instruments are stressed, and in this respect D11 is dedicated to the research of soft condensed matter. D11 underwent a major upgrade in 2008¹. The increased performance of D11 is complemented by dedicated developments for soft matter sample environment², out of which three will be presented here. Of course care has been taken to assure that all developments in sample environment fit onto all three ILL SANS instruments.

First, we will report on a successful in-situ DLS SANS experiment (DLS: dynamic light scattering)³. A combined setup was mounted at D11. Time-resolved studies of processing of nanoparticles for biomedical applications in the cancer therapy could be followed up at different length scales with the dual-beam instrumentation. The structure and shape is elucidated. Concerning time slices, SANS is the faster method, where time slices of 1s and below are feasible. DLS needs at least a measurement time of 10 s.

Second, our tumbling sample rack will be presented. A frequently encountered problem in SANS studies is the instability of liquid suspensions. For solutions containing large particles, the particles often settle down during the time of the scattering experiment. Thus, concentration changes inside the scattering volume make it often difficult to interpret SANS data quantitatively. A six-position changer rack for liquid samples in standard quartz cells has been developed, with the quartz cells rotating at variable speed around the axis of the neutron beam. The copper block containing the cells can be connected to a thermostated bath and allows for temperature control.

Third, we will report on the project of a new pressure cell for the ILL SANS instruments. The new cell will be operating up to 5000 bar, having a path length of 2mm. Temperature control is possible between 0°C and 100°C. The cell will be commissioned in autumn 2012.

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CT29

Polarization analysis with ^3He spin filters to separate coherent scattering from total scattering in SANS

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In soft matter SANS studies, especially at large Q , incoherent scattering becomes the dominant signal. The incoherent contribution can be orders of magnitude larger than the coherent signal of interest; even after the total signal from the solvent is subtracted. This is an intrinsic problem because this remaining incoherent signal comes from the sample itself and would obscure the desired structural information when the coherent scattering level drops far below the incoherent.

Polarization analysis has the potential to fully separate the coherent signal from the incoherent signal and make analysis of difficult samples more certain or even possible at all: one can increase the fidelity of the coherent signal such that weak scattering can still be seen clearly. However, because of inelastic scattering one must be very careful to correctly perform the polarization and detector efficiency corrections if the scattering is desired in absolute units in the large Q -range, where the coherent scattering is one or more orders of magnitude lower than the sample's incoherent scattering. Therefore, we have performed time-of-flight measurements on the SANS diffractometer KWS2 of the JCNS in Garching to look at the amount of inelastic scattering in order to perform this correction accurately.

This presentation will address the issues associated with the correct separation of coherent and incoherent scattering for soft matter samples and propose and describe a method of implementation using ^3He spin filters and future plans at the JCNS. As a demonstration the results of tests measurements on KWS2 will be presented: they show the viability of the method on a protonated α -lactalbumin solution at 2.5% and 0.25% concentrations in a D_2O buffer solution.

CT30

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

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Magnetic layers are the basic building blocks of a large number of magnetoelectronic devices whose performance heavily relies on the morphologies and microstructures of the individual layers and on the coupling between them. These parameters can change during the process of growth. It is hence important for the understanding and optimization of magnetic layers and heterostructures to accurately monitor the magnetic and structural properties during the deposition process. While the structural *in-situ* characterization of thin films during growth by means of electron diffraction, scanning probe microscopy, photospectroscopy and synchrotron radiation is common practice, only few efforts have been made to characterize the evolution of magnetic properties during the deposition of thin magnetic layers [1,2]. In particular, the direct, *in-situ* measurement of the magnetic properties of films using polarised neutron reflectometry is a challenging task. At FRM II, within a collaboration of TU München, Uni Augsburg and MPI Stuttgart, we have designed and commissioned an *in-situ* sputtering facility at the neutron reflectometer REFSANS that allows the growth and monitoring of the magnetic properties of the multilayers *in-situ*. In this contribution, the experimental setup and the first proof of principle results will be presented. One exemplary measurement is shown in Fig. 1.

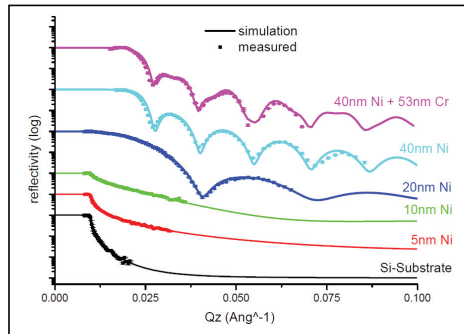


Fig. 1: Typical in-situ reflectivity data obtained using the sputtering facility at REFSANS @ FRM II. The figure shows the reflected intensities as a function of the perpendicular momentum transfer Q_z obtained at different growth steps during the step-wise growth of a Ni/Cr bilayer with final thicknesses of 40 nm Ni + 53 nm Cr on a Si substrate. The reflectivity curves can be fitted using a consistent model where only the layer thicknesses and interface roughness are adjusted.

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CT31

Neutron generation and beam extraction at ESS

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The ESS target monolith will contain the target-moderator-reflector ensemble that generates the thermal and cold neutrons for the beam lines and the first 6 m of the beam extraction and transport systems for the neutron instruments. It is the most safety critical part of the facility and its design needs to be licensed by the Swedish radiation safety authority, SSM. Depending of the design details, more or less of the safety aspects of the target system corresponds to key safety features of nuclear reactors. It is expected though that ESS will be classified as a non-nuclear facility, which will imply savings in time, costs and administrative complexity.

The timeline of the development and construction of the ESS target system contains 3 key milestones. 1) December 2012: completion of the Technical Design Report (TDR), which will serve for closing the design update phase of ESS and starting the realization phase in January 2013. 2) September 2014: completion of the design optimization and engineering design demonstration phase and freezing the design options for subsequent “blue print” design and manufacturing. 3) April 2019: complete installation and operational test without beam and start commissioning and neutron production with beam on target. Routine operation of the target system with fix predetermined schedule is planned to be achieved after 12 months commissioning operation.

The current design baseline for the target systems has been decided by the ESS Steering Committee in June 2012. The optimization and fine tuning of the target design is being pursued under a Change Control procedure, which also contains several interface working groups, including instruments, accelerator, conventional facilities, safety and controls. The conclusions of the working groups and the optimization and design demonstration studies will be implemented as formal baseline changes, wherever needed. Due to radiation damage during operation, the target and moderator-reflector ensemble will be replaced in regular intervals several times within the lifetime of the ESS facility, so the optimization will continue following the medium and long term advances in the field. The main features of the current status of the neutron generation and beam extraction baseline will be presented. This includes the latest update in the optimization of the neutronic performance of the cold moderators, which resulted into a 50 – 120 % gain compared to earlier reference expectations.

Poster

LIST OF POSTER CONTRIBUTIONS / classified by “Discipline”		
Presenting author	Poster number	Discipline: Chemistry Poster number: P01 - P03
Sawinski, H.	P01	Reinvestigating the Crystal Structure of CuNCN
Sawinski, P.	P02	Neutron Powder Diffraction Study on Rubidium Guanidinate, RbCN ₃ H ₄
Widenmeyer	P03	In situ neutron diffraction in the systems V–N and Fe–N
Presenting author	Poster number	Discipline: Condensed Matter Physics Poster number: P04 - P11
Feoktystov	P04	Detailed SANS contrast variation on toluene-based Co ferrofluid
Fu	P05	Coexistence of Novel Magnetic Orders and Spin-glass-like Phase in Pyrochlore Antiferromagnet Na ₃ Co(CO ₃) ₂ Cl
Ruiz-Martin	P06	Study of the Co self-diffusion dynamics in Zr ₂ Co alloy by means of quasielastic neutron scattering
Schindler	P07	Ripening of ZnO nanoparticles studied by SAXS and SANS
Sidoruk	P08	Domain and softmode kinetics in SrTiO ₃ induced by electric fields and mechanical stresses
Szubrin	P09	Electronically induced instabilities in liq. alkali metals
Weber, A.	P10	Towards novel functionalities with metal and complex oxide thin films prepared with molecular beam epitaxy
Xiao	P11	Phase transitions tuned by magnetic field, pressure and chemical doping in EuFe ₂ As ₂
Presenting author	Poster number	Discipline: Geology Poster number: P12 - P14
Randau	P12	First automated pole figure measurements of sample series with a newly developed robot based sample changer system at STRESS-SPEC
Ullemeyer	P13	Texture analysis of polyphase rock samples applying whole pattern deconvolution: methodical aspects
Walter	P14	New Perspectives for In-Situ Fabric Analysis at POWTEX Diffractometer, FRM II, Garching, Germany
Presenting author	Poster number	Discipline: Guide upgrade Poster number: P15
Krist	P15	The neutron guide upgrade project at HZB
Presenting author	Poster number	Discipline: Instrumentation Poster number: P16 - P54 & P90
Clemens	P16	TOF-SANS - from simulation to experiment
Devishvili	P17	SuperADAM: the upgraded polarised neutron reflectometer
Fenske	P18	Small Sample SANS @ ESS
Frontzek	P19	The single-crystal option on the DMC diffractometer
Gan	P20	New measurement options on the stress and texture diffractometer STRESS-SPEC at FRM II
Gilles	P21	SANS-1 – The new Small-Angle Scattering instrument at Forschungs-Neutronenquelle Heinz Maier-Leibnitz
Glavatskyi	P22	Flat-Cone Diffractometer E2 - the power of 3D diffuse scattering for structure solution
Grünwald	P23	KOMPASS - the new triple-axis-spectrometer with spherical polarization analysis to-be at FRM II
Habicht	P24	Performance of the upgraded three-axis spectrometer FLEXX at HZB
Holderer	P25	The Jülich Neutron Spin Echo Spectrometer (J-NSE): Soft Matter in slow motion
Iles	P26	Neutron Laue Diffraction using a Scintillation Plate Detector at HZB
Ioffe	P27	Polarized neutron beam at the SANS diffractometer KWS-2 of the JCNS
Jacobs	P28	POWTEX – High-Intensity Neutron TOF Diffractometer
Kampmann	P29	Perspectives for materials investigations at the Structured Pulse Engineering Diffractometer (SPEED)
Keiderling	P30	New 2D detector of SANS instrument V4 at Helmholtz-Zentrum Berlin
Köhli	P31	The CASCADE Project: Neutron detection using Boron-10 as an alternative to 3He

Krist	P32	Polarizing neutron optics from Helmholtz-Zentrum Berlin
Mattauch	P33	MARIA – The high-intensity polarized neutron reflectometer of JCNS
Meven	P34	Diffraction Studies with Hot Neutrons on HeiDi
Modzel	P35	Jalousie: a highly efficient, large area 10B neutron detector
Pasini	P36	Spin-Echo-Spectrometer Design for ESS
Pipich	P37	Focusing mirror VSANS diffractometer KWS-3: merging nano- and micrometer worlds
Roth	P38	POLI: The new single crystal polarized neutron diffractometer for investigation complex magnetic structures at FRM-II
Rueker	P39	High performance, large cross section S-bender for neutron polarization WITHDRAWN
Russina	P40	Chopper system design for the instruments at pulsed and continuous neutron sources
Schmidt, W.	P41	The upgrade of IN12 Simulations and first neutron measurements
Schrader	P42	The new neutron diffractometer “BioDiff” optimized for crystals with large unit cells at the FRM II
Schulz	P43	Neutron energy analysis by silicon prisms
Schweika	P44	Bispectral powder diffraction at the long pulse source ESS
Skoda	P45	Capabilities and science highlights on the ISIS second target station reflectometers
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Chen	P58	Origin of exchange bias in DyCo/FeNi system
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Presenting author	Poster number	Discipline: Medicine - Pharmacy Poster number: P74
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Presenting author	Poster number	Discipline: Neutron Instrumentation Poster number: P75 -P76
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Nowak	P76	Magnetron sputter deposition of B4C conversion layers for neutron detection
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Presenting author	Poster number	Discipline: Soft Matter Poster number: P79 A - P83
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Presenting author	Poster number	post-deadline poster
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Klobes	P85	Nano- and microstructure of thermoelectric PbTe alloys studied by small angle neutron scattering
Zakalek	P86	Induced Magnetisation in Pd/Fe-Multilayers
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Müller, Th.	P88	Neutron diffraction on highly stoichiometric YFe ₂ O _{4-δ} single crystals
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P01

Reinvestigating the Crystal Structure of CuNCN

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Magnetically active transition-metal carbodiimides have been known for less than a decade. Among these, the phase CuNCN, which may be looked upon as the nitrogen analogue of cupric oxide, CuO, was first synthesized and structurally characterized (space group *Cmcm*) in 2005 [1]. Since then its somewhat mysterious magnetic properties have been under investigation but are far from being fully understood. For example, while the first-order Jahn–Teller distortion found for the nitrogen-coordinated Cu²⁺ ion as well as the magnetic susceptibility allude to antiferromagnetic order between the spin- $\frac{1}{2}$ sites, the first neutron-diffraction studies carried out with the SV7 diffractometer at the DIDO reactor did not show any sign of a magnetic ordering [2]. Likewise, diffraction studies using polarized neutrons by use of the DNS machine at FRM II did not evidence any magnetic Bragg peaks [3].

Herein, we focus on the results of a high-resolution temperature-dependent structural study of CuNCN carried out at the POWGEN instrument at the SNS. Puzzingly enough, the diffraction data clearly manifest a surprising non-monotonous behavior of the *a* lattice parameter as a function of the temperature: its decrease while the temperature lowers turns to a distinguishable increase below 100 K. This effect in the copper spin- $\frac{1}{2}$ system was related to the activated behavior of ESR- and SQUID-measured spin susceptibilities. In addition, an adequate, yet approximate, picture of a two-dimensional resonating valence-bond state has been proposed for CuNCN [4].

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P02

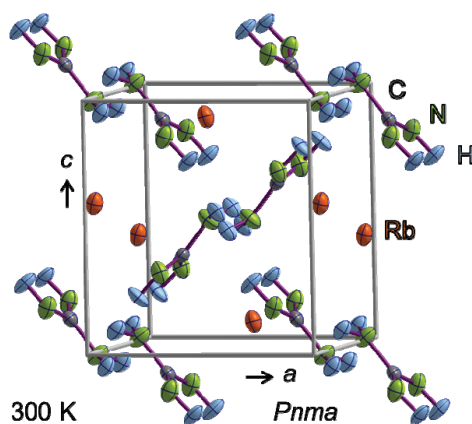
Neutron Powder Diffraction Study on Rubidium Guanidinate, RbCN_3H_4

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Rubidium guanidinate, RbCN_3H_4 , was first synthesized in 2011 through a solid-solid route using molecular guanidine, CN_3H_5 , and rubidium hydride. RbCN_3H_4 is not only the first crystalline salt containing the guanidinate anion, it also represents the archetype of a novel class of compounds. Its structural characterization was based on X-ray powder diffraction (XRPD) data [1], giving access to the positions of the Rb, C, and N atoms, both at room temperature and at 10 K. The hydrogen-atom positions, however, were found from first-principles (GGA) electronic-structure calculations. We here report on neutron-diffraction experiments carried out at 10 K and at room temperature to experimentally corroborate or disprove the theoretical results. It turns out that electronic-structure theory and neutron diffraction are in excellent agreement. We also note that the XRPD-derived structural model suffered from our inability to correctly model the thermal motion of the entire molecular anion, for obvious reasons. Nonetheless, single-crystal X-ray studies on molecular guanidine already indicate that the C–N bond lengths decrease with increasing temperature [2], a phenomenon that may go back to a rigid-body behavior of the organic molecule. For the first time, high-resolution neutron-diffraction data now allow us to determine highly accurate anisotropic displacement parameters for all atoms of the guanidinate complex anion. Based on these results, a new model for the rigid-body movement including a full librational analysis will be presented.



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P03

In situ neutron diffraction in the systems V–N and Fe–N

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For real-time studies of solid-gas reactions aiming for 3d-metal nitrides *in situ* powder neutron diffraction as bulk measurement method in combination with the large scattering length of nitrogen bears ideal conditions to study intermediates and possible formation mechanisms. So far only few setups can face the necessary requirements like chemical inertness, temperature stability and neutron transparency and are well established to realize solid-gas reactions on a neutron diffractometer. A recently presented sapphire single crystal cell for high pressure reactions with hydrogen developed by Kohlmann *et al.* [1] is able to overcome most of those obstacles. Here, we present a newly developed silica glass gas flow cell for solid-gas reactions up to 1275 K, which enable us to study for the formation of vanadium and iron nitrides. The samples are heated contactless and without any parasitic contribution to the patterns by a two-sided laser heating system. Reaction temperatures are monitored by a calibrated pyrometer [2].

The potential of the gas flow cell was tested with an *ex situ* neutron diffraction measurement of δ -VN_{1-x}. The composition was determined by Rietveld refinement to be VN_{0.82(8)}, which is equal to those detected by hot gas extraction technique. Afterwards an *in situ* experiment with vanadium powder in flowing ammonia was performed. At 300 K no reflections are visible, due to a scattering length of vanadium close to zero. At 875 K first reflections of the main product δ -VN_{1-x} appear. Above 925 K β -V₂N_{1-y} is additionally formed. By increasing the temperature up to 1010 K more vanadium is reacted to the mentioned nitride phases. *Ex situ* powder X-ray diffraction of the product shows the presence of a small amount of the nitrogen poor phase V₁₆N_{1.5} [2].

Furthermore, in a second *in situ* experiment iron powder was reacted with flowing ammonia to synthesize different iron nitride phases, γ' -Fe₄N_{1-y} and ε -Fe₃N_{1±x}. The results of full profile Rietveld refinements up to 800 K are in good agreement with data collected by temperature dependent neutron diffraction [3], by *ex situ* powder X-ray diffraction and by thermal analyses. Above 660 K γ' -Fe₄N_{1-y} is present. At 670 K additional reflections, which belong to ε -Fe₃N_{1±x} arise. Above 750 K the ε -phase starts to loose nitrogen. This is also visible in a noticeable shrinking of the hexagonal unit cell, especially of the a -axis. Finally at 800 K the transformation into γ' -Fe₄N is completed [2].

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P04

Detailed SANS contrast variation on toluene-based Co ferrofluid

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Contrast variation is a powerful technique [1], which is widely applied for studies of complex systems in small-angle neutron scattering experiments. The advantage of H/D substitution in the solvent without change in its chemical properties makes it possible to study such many-component systems in detail. In case of polydisperse systems one has to consider averaging of the scattering intensity over the particle size distribution. Direct modeling of the scattering intensities requires a certain number of free parameters (including parameters of the polydispersity function). Large number of local minima of the fit and possible correlation between parameters can give the researcher a wrong conclusion about the structural parameters. Although the data treatment becomes difficult the developed approach of contrast variation for polydisperse systems [2] allows researcher to obtain parameters, which can be later fixed in the model. A successful application of the developed approach in contrast variation on iron oxide magnetic fluids can be found in [3, 4].

In the present work we report about the contrast variation study of cobalt ferrofluid based on toluene with oleoyl sarcosine as surfactant for nanoparticle stabilization. The initial magnetic fluid of 1.2 vol. % of magnetic nanoparticles was diluted with toluene in the ratio 1:5. Several contrasts were prepared so that the amount of deuterated toluene in the solvent varied in the range 0-85%. The corresponding buffer solutions were prepared too and used to subtract solvent background from the sample scattering. Structural parameters of the nanoparticles were precisely obtained and used for further modeling of the scattering curves.

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P05

Coexistence of Novel Magnetic Orders and Spin-glass-like Phase in Pyrochlore Antiferromagnet $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$

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We present comprehensive investigations on a pyrochlore antiferromagnet $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$ [1]. Performed DC susceptibility measurements indicate a broad maximum at around 4 K. The field dependence of the peak temperature of this maximum follows the Almeida-Thouless line, suggesting a spin-glass-like phase transition. The AC susceptibility measurements determine the glassy transition temperature to be 4.5 K and reveal a frequency-independent peak at 17 K. The temperature dependence of the specific heat shows a sharp peak at 1.5 K and a broad hump at around 5 K, which are attributed to a long-range magnetic phase transition and a spin-glass-like freezing process respectively. The average crystallographic structure of $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$ has been determined using neutron powder diffraction. No obvious site disorder has been detected. The diffuse neutron scattering with polarization analysis reveals short-range spin correlations characterized by dominating antiferromagnetic coupling between nearest neighbours and weak ferromagnetic coupling between next nearest neighbours. The long-range magnetic order below 1.5 K is evidenced by the magnetic reflections observed at 50 mK and can be well explained with an all-in-all-out spin configuration. Inelastic neutron scattering of $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$ exhibits spin-wave excitations at 0.5 K, which indicates that the spin-glass-like transition temperature $T_g = 4.5$ K does not correspond to a complete spin-glass freezing as expected in canonical spin glasses. The peak observed in magnetic susceptibility at 17 K is attributed to the onset of an intermediate partially-ordered phase transition, qualitatively consistent with the theoretical predictions for pyrochlore antiferromagnets with weak ferromagnetic next-nearest-neighbour interactions.

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P06

Study of the Co self-diffusion dynamics in Zr_2Co alloy by means of quasielastic neutron scattering

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The single particle dynamics of cobalt within the Zr_2Co melt alloy has been investigated as a function of temperature by means of quasielastic neutron scattering on the time of flight spectrometer TOFTOF, at the Research Neutron Source Heinz Maier-Leibnitz (FRM II).

Due to the high chemical reactivity of the Zr-based alloys, the melts have been containerlessly processed in a compact electrostatic levitation device specially designed for performing neutron scattering experiments [1]. This technique has allowed us to study a broad temperature range, from ~ 1350 K down to temperatures of ~ 1100 K in the metastable regime of an undercooled liquid, below the melting point ($T_m = 1323$ K). Values of the Co self-diffusion coefficients have been determined as a function of temperature by analysing the wave vector dependence of the half widths of the quasielastic lines in the neutron spectra. The values are on the same $D(T)$ curve as the Ni self-diffusivity values measured recently for melts of $\text{Zr}_{64}\text{Ni}_{36}$ [2] and as the mean Ni and Ti self-diffusivity values in melts of glass forming $\text{Zr}_{41.2}\text{Ti}_{13.8}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$ [3]. This suggests similar mechanisms of transition metal self-diffusion in all three liquids.

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P07

Ripening of ZnO nanoparticles studied by SAXS and SANS

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ZnO semiconductor nanoparticles (NPs) exhibit promising electro-optical properties for applications in e.g. solar cells or light emitting devices due to the quantum size effect. Thus, the preparation of well-defined, stable ZnO-NPs is of high interest and therefore knowledge about the nucleation and growth processes is crucial.

The synthesis is carried out in ethanol using equimolar solutions of zincacetate and lithiumhydroxide which are simply mixed. The nucleation of the NP occurs instantly, while a further ripening of the ZnO-NPs starting from about 2 nm as a function of temperature can be observed using UV/Vis measurements or transmission electron microscopy (TEM). Cooling to -10°C immediately after the synthesis results in stable particle sizes for months, while at a temperature of 40°C ripening to sizes of 6 nm was observed at a timescale of several hours.

This ripening process is investigated using temperature and time-dependent SAXS measurements. Using a triaxial ellipsoid as model the X-ray data of the ZnO-NPs could be well described. However, including an acetate layer around the NPs did not change the fit demonstrating SAXS to be not sensitive to the organic stabiliser. Thus SANS measurements were conducted to get insight into the structure of the stabilizing layer self-assembled around the ZnO Nps. Also structural changes of the stabilizing layer during particle growth will be addressed.

P08

Domain and softmode kinetics in SrTiO₃ induced by electric fields and mechanical stresses

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Strontium titanate (SrTiO₃) is a well-known member of the perovskite family. It exhibits an antiferrodistortive phase transition at 105 K leading to a tetragonal paraelectric phase with three different structural domains. At low temperatures a polar phase can be induced by the application of electric field [1].

Surprisingly, the domain distribution can be changed by applying uniaxial mechanical stress as well as electric field, although a direct coupling between the order parameter and the electric field is forbidden by symmetry [2].

Therefore, we quantitatively determined the domain distribution in a single crystal of SrTiO₃ by neutron diffraction using different instruments at FRM II and ILL. Careful determination of the intensities of tetragonal superlattice reflections allowed us to observe the variations of domain volume fractions as a function of applied stress and electric field along different crystallographic directions. It is shown that stress and electric field exhibit competing effects and the proximity of the field induced ferroelectric phase plays an important role. Moreover, real time stroboscopic elastic and inelastic experiments allowed us to determine the kinetics of the domain redistribution and of the softmode transition to the ferroelectric phase in detail. These investigations provide a basis for the understanding of the basic microscopic mechanisms.

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P09

Electronically induced instabilities in liq. alkali metals

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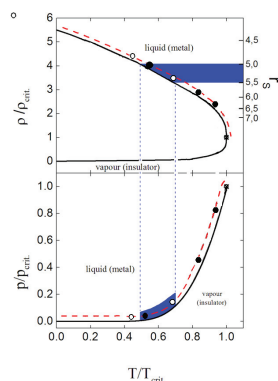
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Quantum mechanical calculations of the ground state energy for a pure electron gas at different densities reveal a thermodynamic instability in terms of a negative compressibility [1] if the gas is expanded to values where the Wigner-Seitz Parameter is $r_s \approx 4.5$ -5, if r_s is given in units of the Bohr radius. We have investigated this feature exploring fluid alkali metals which appear to be perfect model systems for this purpose. Their electronic properties can be well described within the free-electron approximation and their ion density and hence their electronic density can be gradually reduced along the liquid vapour coexistence line (indicated by the red dashed lines in the Figure).

Appropriate scaling of r_s [2,3] reveals that the predicted instability should occur at about four times the critical density in these systems (≈ 1200 K, ≈ 25 bar in liquid Rb).



Reduced alkali metal phase diagram in the density-temperature and in the pressure-temperature projection. T_{crit} and p_{crit} are critical temperature and pressure, respectively. Shaded areas represent density range of the predicted instability. Points correspond to measured states

Estimates of the thermodynamic stability employing equation of state data for Rb and Cs (see [2] and references therein) show indeed that the stability criteria seems to be violated when these fluids are expanded beyond this density range (blue shaded areas in Fig. 1) The liquid state however, persists to even lower densities and the electrical conductivity is still relatively high. The occurrence of a negative compressibility also causes a negative dielectric constant of the electron gas. This however, would lead to drastic variations in the interparticle interactions and should hence be reflected in structure and dynamics of the fluid. Such structural variations were recently observed in a series of highly accurate $S(Q)$ -measurements on liquid rubidium [3], but this effect must also lead to a variation of the mode frequencies of the collective dynamics. In order to investigate this, we have measured $S(Q, \omega)$ of fluid Rubidium at lower Q values for a variety of thermodynamic states close to the vapour pressure curve at temperatures between melting and 1873 K. For this we have used the small angle capabilities of the instruments BRISP and IN4 which are

located at the High-Flux-Reactor of the ILL in Grenoble.

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P10

Towards novel functionalities with metal and complex oxide thin films prepared with an oxygen assisted molecular beam epitaxy

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At the Jülich Centre for Neutron Science (JCNS) a state-of-the-art oxide-MBE system was commissioned in 2010. Up to now we managed to produce thin metal and oxide films in single layers as well as multilayers with high crystalline quality and very little roughness.

Here we present the results on patterned magnetic structures of Fe/Cr multilayers and on unstructured, ultrasmooth LaMnO₃/SrMnO₃ (LMO/SMO) multilayers. Both systems were characterized magnetically with SQUID magnetometry and Neutron reflectometry with full polarization analysis.

In the Fe/Co multilayers the Cr interlayers induce an antiferromagnetic coupling between adjacent Fe layers. Thus, the magnetic dipole moment is reduced and a magnetic superstructure is created, which is, due to the contrast of Cr to Fe, easily observable by polarized neutron reflectometry. The lateral structuring was performed by UV-nanoimprint lithography and reactive ion etching. The structural characterization was carried out by scanning electron microscopy, atomic force microscopy and X-ray scattering under grazing incidence. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. Polarized neutron reflectometry and off-specular scattering was used to determine the magnetic domain formation within the individual layers which gives insight into the interplay of the shape and the crystalline anisotropies.

The LMO/SMO multilayers show an interface induced ferromagnetic behavior within the LMO in contrast to the antiferromagnetic behavior of the single layers. We carried out a thickness dependent study of the magnetic moment induced by the interfaces with SQUID magnetometry. To study the depth resolved magnetization profile we will measure several multilayers with varying interlayer thickness on D17 at the ILL in September. We will include these results in this presentation.

In future we want to study metal and complex oxide films quasi in-situ with neutron scattering at the MAgnetism Reflectometer with high Incident Angle (MARIA) of the JCNS at FRM II. For this purpose a transport chamber is under construction and the MBE system will be accessible for users.

P11

Phase transitions tuned by magnetic field, pressure and chemical doping in EuFe_2As_2

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The study of phase transitions tuned by experimental control parameters, such as magnetic field, pressure and chemical substitution, is a field of great interest. Among various iron pnictide parent compounds, EuFe_2As_2 stands out due to the presence of both spin density wave of Fe and antiferromagnetic ordering of localized Eu moment. The effects of magnetic field, pressure and chemical doping on the magnetic and structural properties of EuFe_2As_2 have been investigated by using neutron diffraction and various macroscopic characterization techniques.

A field-induced spin reorientation is observed in EuFe_2As_2 with the presence of a magnetic field along crystallographic axes. Interestingly, the existence of giant spin-charge-lattice coupling is verified as indicated by the redistribution of twin population and anomalous in-plane magnetoresistance. Upon chemical doping on EuFe_2As_2 parent compound, e.g. P doped on As site or Co doped on Fe site, it was found that antiferromagnetic spin configuration of Eu changes to incommensurate ordering state due to the modified RKKY interaction, while the application of pressure up to 25 kbar can hardly change the ground-state antiferromagnetic spin configuration of Eu although it can suppress the spin density wave order of Fe and induce the superconductivity in EuFe_2As_2 .

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First automated pole figure measurements of sample series with a newly developed robot based sample changer system at STRESS-SPEC

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After the ending of the moratorium about the exploration of Gorleben for a potential nuclear waste disposal site, an increasing scientific interest exists, to understand the evolution of salt diapirs. To understand the internal kinematics of these salt diapirs, natural samples as well as experimentally deformed salt samples from controlled deformation parameters have to be investigated. On that account a thermo mechanical apparatus was developed for experimental phase specific deformations of rock salt (Zulauf et al., 2007, 2009). In this study composite natural samples, consisting of a single layer of anhydrite embedded in halite matrix, were coaxial deformed.

The deformation of this halite in samples from Asse reveals two plateaus in the stress-strain plot. The first one is at about 5 % strain and the second one seems to terminate the strain hardening effects observed at 25 % strain. It is proposed, that these effects are related to different sets of active glide systems during deformation. This can be systematically revealed by texture analysis.

For texture investigations of this kind of coarser grained materials as it often occurs in geological sample it is problematic to achieve enough grains for an acceptable grain statistic. Through the combination of a newly developed sample changer and the continuous pole figure measuring method it is possible to increase the investigated gauge volume of this coarse grained salt samples, by measuring more than 40 subsamples. We will present the first texture results of the combined data and the capability of this newly developed robot based sample changer system at STRESS-SPEC (Brokmeier et al., 2011).

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P13

Texture analysis of polyphase rock samples applying whole pattern deconvolution: methodical aspects

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Texture analysis of polycrystals is usually performed on a small number of diffraction pole figures. This is impractical for many polyphase rock samples, because the diffraction patterns are often complicated with many peak overlaps. In such cases the concept of RIETVELD structural refinement can be combined with texture analysis leading to the possibility to determine crystal structure, texture and residual strain simultaneously [1] [2]. Particular algorithms for the so-called 'Rietveld texture analysis' (RTA) are meanwhile available [3] [4]. However, despite obvious advantages of RTA, there are limitations like counting statistics, grain statistics, resolution, accessible d - range and so on. In addition, specific properties of the basic experimental method may apply. The TOF neutron spectra we are dealing with in the following are characterized by non-uniform counting statistics, because the intensity of the diffracted beam and the intensity distribution of the reactor spectrum depend on the wavelength of the neutrons. Methodical investigations to ensure reliability of the results obtained from RTA and to determine the optimal experimental conditions appear to be appropriate.

Three samples consisting of forsterite (sample 1), quartz (sample 2) and calcite+dolomite (sample 3) were measured at the SKAT texture diffractometer in Dubna [5] and the mineral textures were determined by means of RTA applying the MAUD algorithm [3]. Subsequently, an artificial sample was created by simply summing up the spectra of the three samples leading to many peak overlaps especially at small d - spacings. RTA was applied to this data set and the resulting textures were compared to the former textures, which are assumed to represent the better results, because they were determined from spectra without overlapping Bragg reflections. No significant differences between particular mineral textures could be detected. Even variation of the d - range considered for the texture evaluation and thinning out the measuring grid to some extent had no significant effect. We conclude that RTA is a reliable tool for texture determinations on polyphase rock samples with comparable sample state. Whether this conclusion is valid for even more complicated samples (more phases / lower lattice symmetry) must be proven.

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P14

New Perspectives for *In-Situ* Fabric Analysis at POWTEX Diffractometer, FRM II, Garching, Germany

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Fabric analysis is in geo- and materials science a basic tool for understanding deformation and recrystallisation processes and for the quantitative characterisation of the anisotropic physical properties of (rock) materials. Neutron texture diffraction is especially useful for geoscientific sample material, as larger sample volumes of often heterogeneous and coarse-grained material, can easily be measured in statistical sufficiency due to the high penetration capabilities of neutrons.

The new POWTEX (POWder and TEXTure) Diffractometer at the neutron research reactor FRM II in Garching, Germany is designed as a high-intensity diffractometer by groups from the RWTH Aachen, Forschungszentrum Jülich and the University of Göttingen (Houben et al. 2009). Complementary to existing neutron diffractometers (SKAT at Dubna, Russia; GEM at ISIS, UK; HIPPO at Los Alamos, USA; D20 at ILL, France; and the local STRESS-SPEC and SPODI at FRM II) the layout of POWTEX is focused on fast time-resolved experiments and the measurement of larger sample series as necessary for the study of large scale geological structures. POWTEX is thereby also a dedicated beam line for geoscientific research. Due to the detector design and coverage of ~ 10 sr, the TOF technique and the optimization to high flux ($\sim 1 \times 10^7$ n/cm²s) at the sample, effective texture measurements without sample tilting and rotation are possible. Furthermore, the instrument and the angular detector resolution is designed also for strong recrystallisation textures. These instrument characteristics therefore allow *in-situ* time-resolved texture measurements during deformation experiments on rocksalt, ice and furthermore *in-situ* recrystallisation experiments as large sample environments will be implemented at POWTEX by the group of the University of Göttingen.

The *in-situ* deformation apparatus is operated by a uniaxial spindle drive with a maximum axial load of 200 kN, which will be redesigned to minimize shadowing effects inside the cylindrical detector. The HT deformation experiments will be carried out in uniaxial compression or extension and an upgrade to triaxial deformation conditions is envisaged. The load frame can alternatively be used for ice deformation by inserting a cryostat cell for temperatures down to 77 K with a triaxial apparatus allowing also simple shear experiments on ice. Strain rates range between 10^{-8} and 10^{-3} s⁻¹ reaching to at least 50 % axial strain. The deformation apparatus is designed for continuous long-term deformation experiments and can be exchanged between *in-situ* and *ex-situ* placements during continuous operation inside and outside the neutron detector.

The furnace for the 3D-recrystallisation analysis of single grains will be realized complementary to the furnace that already exists for fine grained materials at the synchrotron beamline BW5 at HASYLAB, Germany (Klein et al. 2009, and references therein).

It will be a laser mirror furnace with temperatures up to 1800° C, which will be rotatable around a vertical axis to obtain the required stereologic orientation information.

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P15

The neutron guide upgrade project at HZB

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The Helmholtz-Zentrum Berlin has exchanged its cold source. At the same time the complete neutron guide system from the extraction part to the instruments in neutron guide hall 1 was rebuilt.

The state-of-the-art neutron guide system was designed using advanced neutron optics in order to fully exploit the new cold source and to reduce the beam losses during transport. Most guides are coated with $m=3$ supermirrors.

In this process an additional guide was created which will be used as a test beam line for the ESS upgrade project.

The change of the guide system offered the unique chance to relocate some of the instruments and bring them to optimal positions. Especially the cold triple axis instrument FLEX will profit from an end position and the cold time-of-flight instrument NEAT will have an extended flight path ending in a new building.

Since the total guide cross section is doubled and the guide coating is changed from ^{58}Ni to supermirrors with $m=3$ the radiation has strongly increased. Based on MCNP calculations a shielding system was designed which is close to the neutron guides and consists of a sandwich to ensure that the former radiation levels are kept.

P16

TOF-SANS - from simulation to experiment

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VSANS/V16 is the second small-angle neutron scattering instrument at BER-II. In contrast to the other user instrument V4, which works in constant wavelength mode and with a polarized neutron beam option, the new instrument is dedicated to serve solely the soft matter community and performs time-of-flight (TOF) mode measurements. VSANS/V16 allows for pinhole camera set-up between 1 and 12 m collimation length as well as for a multi-pinhole set-up that extends the usually accessible range of momentum transfers to 0.001 nm^{-1} . Within the VITESS simulation software package, we found optimized chopper parameters and could program the scattering experiment for a subsequent comparison to the real data. This procedure helps to identify the necessary instrument lay-out for an individual user experiment. In order to test the simulation and the TOF experiments, we established a way of reducing the TOF-data from a pinhole camera set-up within the framework of the MANTID software package and compared the results to measurements taken on V4 for monodisperse latex spheres. The analysis shows comparable results at very good agreement with the advantage of enhanced resolution in the case of V16 above 0.1 nm^{-1} .

In a second part we present the Rheo-SANS option of V16 based on a commercial rheometer that will be incorporated into the control software and whose data will be synchronized to the event recording data acquisition system. With the help of this option we will be able to connect rheometric data with structural data from small-angle neutron scattering.

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SuperADAM: the upgraded polarised neutron reflectometer

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A new neutron reflectometer SuperADAM has recently been built and commissioned at the Institut Laue Langevin, Grenoble, France. The instrument features two modes of operation: a high resolution polarised option and a high flux mode. The high resolution mode uses a solid state polariser/wavelength filter providing a highly polarised (up to 98.6 %) monochromatic neutron flux of $8 \cdot 10^4 \text{ n} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ with monochromatisation $\Delta\lambda/\lambda = 0.7 \%$ with divergence $\Delta\alpha = 0.2 \text{ mrad}$. The high flux option provides a flux of $1.4 \cdot 10^6 \text{ n} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ with a relaxed wavelength resolution of $\Delta\lambda/\lambda = 2.2 \%$ with $\Delta\alpha \approx 0.6 \text{ mrad}$. The instrument includes both single and position sensitive detectors. Polarisation analysis can be performed with a wide angle solid state analyser[1] or with ^3He spin filter cell. High efficiency detectors, low background and high flux provides a dynamic range of up to seven decades of reflectivity which significantly broadens the scientific application range of the new instrument. The detailed specifications and the instrument capabilities are illustrated with examples of latest scientific highlights[2-4].

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P18

Small Sample SANS @ ESS

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SANS instruments with neutron beam cross sections in the range of $2 \times 2 \text{ mm}^2$ or down to a few $10 \times 10 \text{ }\mu\text{m}^2$ are strongly requested in biology as well as in soft matter research and material science. The small cross sections enable new SANS measurements which are generally only be performed at synchrotron source (SAXS), e.g. the scanning of domains in microstructured materials or the analysis of smallest sample volumes. A challenge of the small dimensions is the neutron flux. For a sample size of about $50 \times 50 \text{ }\mu\text{m}^2$ the scattering volume and associated with it the intensity would be reduced by an order of about 5 compared to conventional samples sizes.

The expected high flux and the time structure of the proposed long pulse neutron spallation source ESS offer the opportunity for such measurements. The neutron flux, however, has to be focused on the sample to compensate for the smaller volume. At the same time the background has to be minimized to increase the signal to noise ratio. The focusing of the neutron flux not only increases the intensity on the sample but due to Liouville's theorem also increases the divergence.

Here we present a conceptual design for an optimized small sample SANS instrument at the long pulsed spallation source ESS (see fig. 1). McStas simulations have been used to compare the performance of different SANS concepts. In particular the focusing options and devices as, for example, parabolic and elliptical neutron guides have been analyzed. Furthermore the performance of a multiple beam set up [1] has been investigated to tune the divergence and the accessible Q-range.

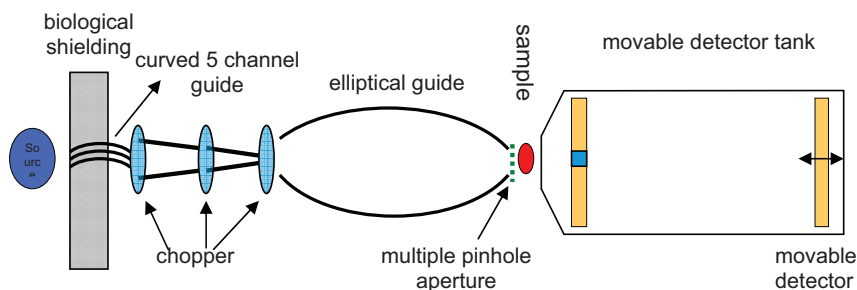


Fig. 1: Conceptual Design of the small sample SANS instrument at ESS

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P19

The single-crystal option on the DMC diffractometer

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The DMC at the SINQ neutron source is a cold source neutron powder diffractometer featuring a “banana” type multi-detector (a schematic sketch is shown in Fig. 1). Recent improvements lead to a very low, stable and uniform background. The super-mirror guide gives a relative high flux of cold neutrons at the sample position.

The features of the instrument make it extremely well suited also for single crystal diffraction experiments. The rotation of the single crystal allows to measure full-reciprocal planes in one orientation. The information contained in these data can lead to a deeper understanding of, for instance, the inherent magnetic structure. Especially, in cases of frustrated magnetism and the resulting low-dimensional or short-range ordered magnetic structures these full-reciprocal planes often allow an assessment of the anisotropy of these structures and subsequently of magnetic correlations. The low and uniform background especially helps to identify diffuse scattering.

The search for unknown magnetic correlations and structures is aided by the vast possibilities of sample environments allowing milli-Kelvin temperatures and moderate magnetic fields (planned upgrades on the instrument will allow high magnetic fields).

In our contribution we will present a detailed instrument description as well as single crystal data from DMC on two show cases. In Tb_3Co multiple magnetic structures are realized in a small temperature-field area around the ordering temperature. We will show that the data from DMC allows the precise identification of the different magnetic phases. In Ho_2PdSi_3 strong diffuse magnetic scattering is found as a precursor to the magnetic structure. Here, the data allows the assignment of a commensurate propagation vector even in the paramagnetic state.

We hope that our contribution will advertise DMC to the neutron-scattering community as a powerful single crystal diffractometer, especially suited for the investigation of low-dimensional magnetism and short-range ordered phenomenon.

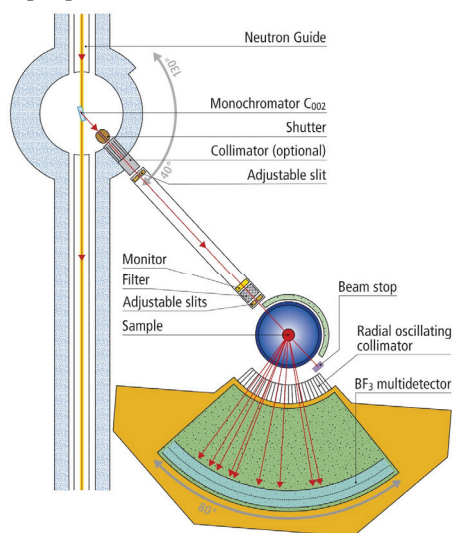


Fig. 1: schematic sketch of the DMC instrument

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New measurement options on the stress and texture diffractometer STRESS-SPEC at FRM II

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STRESS-SPEC is a high flux neutron diffractometer and offers a flexible instrument setup suitable for fast residual strain and texture (bulk, local or gradient) measurements [1, 2]. Recently pole figure measurements have been speeded up due to a new 2D detector with higher efficiency and larger area. In addition, a robot system allows automatic and precise sample change and positioning for global texture analysis which greatly improves the efficient use of beam time. Furthermore the available test rig was upgraded to facilitate in-situ strain and FWHM pole figure measurements under uniaxial load and /or compression [3].

Here we present the implementation of the new robotic technique at STRESS-SPEC (supported by BMBF project) and will show as a case study recent results of texture analysis on deformed coarse grained salts using the robot sample changer system. Besides that in-situ pole figure measurements on a steel using the upgraded tensile rig will also be presented.

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P21

SANS-1 – The new Small-Angle Scattering instrument at Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

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A new small-angle scattering instrument SANS-1 is installed on beam line NL 4a at the Heinz Maier-Leibnitz Forschungs-Neutronenquelle (FRM II). It is a joint venture of the TU München and the Helmholtz Zentrum Geesthacht (HZG). SANS-1 is optimised to be one of the most intense and versatile small-angle scattering instruments with an outstanding range in momentum transfer and dynamic range [1]. SANS-1 is dedicated for investigation of material science and magnetism, both in basic elementary research and applied sciences. The instrument was designed using the program McStas to optimise the dimensions and the features of the different optical components [2] within the boundary conditions given by the provided space and interaction with neighbour instruments. The SANS-1 instrument is currently in the commissioning phase.

Together with the detector group of FRM II an exposure on the 1m² detector was performed to get a first impression of the beam quality. A sample of Silver behenate powder [CH₃(CH₂)₂₀COOAg] was used [3], providing cold neutron Bragg reflections in the angular range of 4-26°. A full diffraction pattern of the corresponding Debye-Scherrer rings was recorded on the large detector. Afterwards a calibration on each of the 128 tubes concerning position and efficiency was performed. It is planned to measure with friendly users in the period of autumn up to the end of the year. Adjacent first users will be served with beam time.

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P22

Flat-Cone Diffractometer E2 – the power of 3D diffuse scattering for structure solution

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The Flat-Cone E2 is a medium resolution single crystal and powder diffractometer, providing the wide sample environment possibilities to study the complicated distributions of Bragg and superstructure reflections in three dimensions of reciprocal space (Flat-Cone), low intensity sublattice scattering patterns and diffuse scattering arising from structural and magnetic disorder.

A 3-dimensional part of the reciprocal space can be scanned in few steps by combining the “off-plane Bragg-scattering” and the flat-cone layer concept while using a computer-controlled tilting axis of the detector bank. Parasitic scattering from cryostat or furnace walls is reduced by an oscillating “radial” collimator. The special software package TVneXus deals with raw data sets, transformed physical spaces and usual data analysis tools (e.g. MatLab). TVneXus can be used to convert various data sets e.g. into powder diffractograms, linear detector projections, rotation crystal pictures or the 2D/3D reciprocal space.

We represent some most interesting examples of the 3D diffuse scattering studies utilizing the power of Flat-Cone for the crystal and magnetic structure solution in complicated cases, like:

- short-range ordered planar defect network in a self-accommodated ferromagnetic martensite of Ni-Mn-Ga shape memory alloys [1-2] and sodium cobaltate [3];
- frustrated antiferromagnets [4];
- D₂O ice and spin-ice [5].

A 3D reciprocal space studies are proved to be ultimate tool in studies of the magnetic, crystal and defect structure and phase transitions in the crystalline materials, i.e.: One Technique for Different Compounds.

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P23

KOMPASS – the new triple-axis-spectrometer with spherical polarization analysis to-be at FRM II

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KOMPASS, the new, cold neutron triple-axis-spectrometer to-be installed at the FRM II, is fully designed to work exclusively with polarized neutrons and to provide a zero-field spherical polarization analysis. The instrument is therefore dedicated to study all types of magnetic ordering and excitations.

Besides a global presentation of the instrument design, here we will focus on the highlight of the instrument – the state-of-the-art polarizing and parabolically focussing guide system concept, which is expected to provide high polarization rates and a superior flexibility with respect to the resolution in energy and momentum over the conventionally straight, or elliptical, guide systems [1].

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Performance of the upgraded three-axis spectrometer FLEXX at HZB

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The cold triple axis spectrometer FLEX [1] has had a very successful 15 years of operations, serving as a platform for the development of the neutron resonance spin echo (NRSE) technique [2,3] in addition to being popular with the user community [4-6] for its ability to exploit the large variety of sample environments available for neutron scattering at HZB. These include the unique combination of high magnetic fields (up to 17 T) and low temperatures (with dilution cryostats down to 30 mK). Recently, the primary spectrometer was upgraded with new $m = 3$ guides with a converging elliptical section to focus neutrons onto a virtual source, which is subsequently imaged on the new double focussing monochromator, ensuring an increase in the neutron flux. In addition, there is a new velocity selector to remove higher order scattering, eliminating the need for filters. A polarising S-bender placed before the elliptical guide section can be vertically moved into the primary beam resulting in higher polarised neutron flux delivered to the sample. This will be useful for the upgraded NRSE option which has been very recently commissioned. We present first experimental results from the upgraded instrument which confirm overall large intensity gains ranging from 2 to 10 as predicted in the design phase from Monte Carlo simulations and analytical considerations. After commissioning the triple-axis spectrometer FLEXX is now back in routine user operation.

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P25

The Jülich Neutron Spin Echo Spectrometer (J-NSE): Soft Matter in slow motion

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Neutron spin-echo (NSE) spectroscopy is the neutron scattering technique with the highest energy resolution down to the sub- μeV range, making it possible to investigate very slow dynamic processes in soft matter systems. Accessible time and length scales (nanometers, nanoseconds) are relevant for observation of thermal fluctuations in mesoscopic systems. High energy resolution, low background and good instrumental stability of J-NSE spectrometer at FRM II research reactor in Garching makes the instrument suitable for very low intensity experiments, as has been shown recently with experiments under grazing incidence (GINSES) [1]. Scientific applications of J-NSE instrument include dynamics of classical and critical microemulsions, microgels, polymer blends, polymers in solution and different confinement, membranes and much more. Some examples of recent experiments will be presented.

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P26

Neutron Laue Diffraction using a Scintillation Plate Detector at HZB

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Neutron Laue Diffraction is an important method of neutron scattering for measuring single crystals. Utilising a white beam consisting of a range of wavelengths, Laue diffraction patterns can be generated in a matter of seconds from very small crystals i.e. $<1\text{mm}^3$. The Laue instrument produces a 2D projection of a large volume of reciprocal space in a single Laue pattern. A Laue Diffractometer is currently under construction in the Experimental Hall at the Berlin research reactor, BER II, at the Helmholtz Centre Berlin for Materials and Energy (HZB). Utilising a direct beam from the D1S beamtube the instrument will sit just 7m from the 10MW neutron source providing a high-flux, uninterrupted neutron beam approximately 10mm in diameter. A scintillating plate detector will 'orbit' the sample whereby two separate plates can rotate from close to back-scattering through 120° to the transmission position. Such rotation will allow a full mapping of the Laue reflections to be constructed. Each plate will be coupled to 4xiCCD cameras, in a similar arrangement to that utilised by CYCLOPS at the ILL [1] providing fast readout time and zero deadtime between measurements.

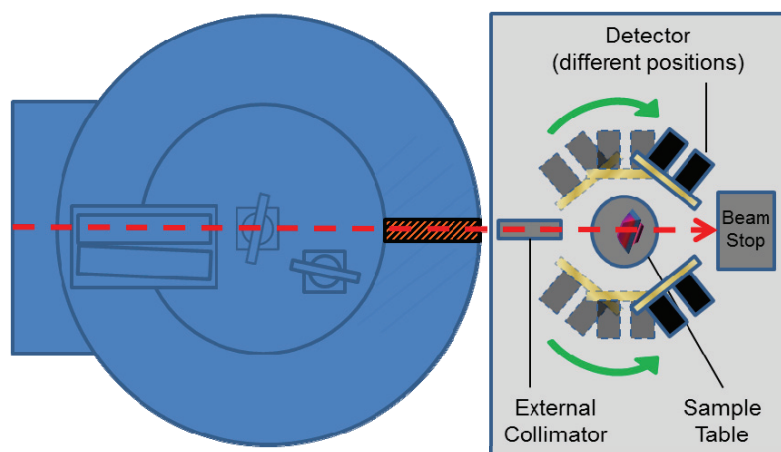


Fig.1: Red-dotted line shows path of neutrons from D1S beamtube, through monochromator shielding of instruments E7 and E10, to the Laue Diffractometer, E11.

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P27

Polarized neutron beam at the SANS diffractometer KWS-II of the JCNS

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We will report on a new development at the high-intensity SANS diffractometer KWS-II of the Jülich Centre for Neutron Science that has been equipped with the transmission polarizer [1] built in the collimation base of the instrument rather close to the sample position. As the sample size is typically $1 \times 1 \text{ cm}^2$, the effective cross-section of the polarizer is rather small ($22 \times 22 \text{ mm}^2$). The polarizer is made of a single plate of super-mirror coated thin Si wafers, resulting in a low attenuation of the neutron beam and is immersed in a strong, 1.4T, magnetic field to suppress the diffuse scattering with the flipped polarization [2].

The polarizer, which has been characterized by means of a ^3He neutron spin filter, provides a high neutron polarization over the whole wavelength range and all incident beam collimations available at KWS2 (92 % at 4.5 \AA and above 99 % for $(6 \div 20) \text{ \AA}$).

Together with an extremely high intensity, such highly polarized neutron beam at a SANS instrument opens exiting opportunities for condensed matter investigations. It will also make the separation of coherent/incoherent scattering from non-deuterized biological molecules (which allows for the observations of a weak coherent scattering at 100 times stronger incoherent background [3, 4]) an experimental routine.

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P28

POWTEX – High-Intensity Neutron TOF Diffractometer **P. Jacobs¹, A. Houben¹, W. Schweika², J. Walter³, H. Conrad², P. Müller¹, B. T. Hansen³, Th. Brückel² and R. Dronskowski¹**

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The POWTEX instrument (POWder & TEXTure acronym) will provide chemists and geo-scientists with a powerful tool for rapid powder and texture diffraction. POWTEX will be installed at FRM II and is designed and built by RWTH Aachen University and Forschungs-zentrum Jülich. Additionally, Göttingen University will provide texture analysis and sample environments. Both projects have been granted by the German Federal Ministry of Education and Research (BMBF). POWTEX's design combines several new concepts [1]. The neutron-guide system consists of two double-elliptic parts with a common focal point of $1 \times 1 \text{ cm}^2$ at the pulse-chopper and sample positions. Hence, the common focal point is an "eye of a needle" in time and space, optimizing time resolution and reducing the source background. The second neutron guide will have an octagonal cross section which, combined with the graded super-mirror coating, results in a Gaussian intensity and divergence distribution [2].

The neutron-guide and the chopper-system components have been ordered and are under construction. Due to the ^3He shortage, two new detector developments were initiated (^6LiF -WSF and ^{10}B -solid-state), built and also tested. The detector design will cover a huge solid angle ($\approx 10 \text{ sr}$) and will allow for large sample environments, e.g., a unique uniaxial and triaxial deformation apparatus developed by the Göttingen group. The large angular coverage is important for texture measurements (*in situ* deformation, annealing, simultaneous stress and texture measurements) because it avoids any need for sample tilting and rotation. For powder diffraction, the covered solid angle relates directly to the instrument's efficiency.

We are presently developing a novel Rietveld code which refines the two-dimensional (2θ , λ) diffractograms and, hence, benefits from the larger resolution in back-scattering mode as well as the high intensity at lower angles. High intensities will not only allow for short measurement times and a large sample throughput, they will also give access to *in situ* chemical experiments, e.g., to characterize phase transitions as a function of T , p and B_0 .

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P29

Perspectives for Materials Investigations at the Structured Pulse Engineering Diffractometer (SPEED)

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One important goal of modern engineering investigations is to improve our understanding of materials behaviour and failure on a microstructural basis. Various experimental investigations are performed to achieve this goal comprising measurements of stresses and textures. Those characterizations need neutron measurements if well defined gauge volumes located deep in the bulk of materials are to be analyzed. Complementary investigations are performed with X-rays to characterize surface structures or to investigate lightweight structures with hard X-rays. Neutron investigations should allow for three-dimensional maps of stresses and textures within engineering components or in-situ studies of fatigue behaviour or stresses in rotating machinery. Those measurements are, however, extremely time consuming and can thus not be performed to the required extent at modern instruments such as SALSA at ILL or STRESS-SPEC at FRM II. New perspectives for engineering applications will be offered by new instruments at MW spallation sources such as VULCAN at SNS.

Against this background the Helmholtz-Zentrum Geesthacht proposes to build a novel structured pulse engineering diffractometer (SPEED) at the European Spallation Source (ESS) in Lund/Sweden. The instrument will be based on a novel ToF-design distinguished by a modulation chopper positioned at a distance of ~ 25 m from the source. This chopper will be located ~ 50 m from the sample and allows setting the wavelength resolution almost independently of the wavelength in a broad range from about 0.15% to 2%. Despite the high resolution the chopper system in total has a transmission of about 30% of the 2 ms long source pulses for a broad and selectable wavelength range. SPEED thus will make full use of the high flux of the long pulse spallation source for high resolution diffractometry from samples of high symmetry. Samples of low symmetry can be investigated by replacing optionally the modulation chopper by another one with less slits. The design of SPEED is introduced and its performance based on numerical simulations for texture and stress measurements is outlined. The development of SPEED is performed as an in-kind contribution to the ESS instrumentation, it is part of the German support to the ESS Pre-Construction Phase and Design Update.

P30

New 2D detector of SANS instrument V4 at Helmholtz-Zentrum Berlin

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The V4 SANS instrument is currently being upgraded with a new large 2D detector, replacing the previous LETI-type multi-wire proportional chamber. The new detector consists of an array of 112 linear position sensitive ^3He -filled tubes with 8 mm diameter from company Reuter-Stokes [1]. Three different tube lengths of 1000 mm, 864 mm and 610 mm are utilized to maximize the detection area within the circular cross-section of the existing detector container. The detector is equipped with 3 movable beam stops. A built-in elevator allows a detector lift of 150 mm at the front position closest to the sample to increase the detected range of the scattering vector Q , and a detector lift of a few mm at all other positions for fine-adjustment of the tubes relative to the beam axis. The mechanical design has been developed at Helmholtz-Zentrum Berlin. The detector electronics and the interface are supplied by Mesytec [2]. They allow for event recording in time-stamp mode where each detected neutron, chopper pulse or any other event is stored with precise time information (100 ns LSB) in a binary file. Any correlation in time between these events can be made offline; wrong data may be filtered out. This option is inevitable, amongst other applications, for the new time-resolved TISANE technique that was recently set up at the V4 instrument [3,4], allowing the investigation of kinetic processes in the microsecond range. The poster presents an overview of the detector design, figures of merit, and first test results.

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P31

The CASCADE Project: Neutron detection using Boron-10 as an alternative to Helium-3

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So far for the efficient detection of thermal neutrons Helium-3 based detectors are used, wherein ^3He serves as a neutron converter as well as a counting gas. The globally increased demand along with the limited availability for this gas asks for the development of alternative technologies.

The research of the Heidelberg instrumentation group aims for the development of such novel systems, which are used for the high rate capable, 2D spatially resolved detection of thermal neutrons. The CASCADE detector [1] presented in this talk uses up to ten with solid ^{10}B coated Gas Electron Multiplier (GEM) foils [2], which serve both as a neutron converter and as an amplifier for the primary ionization deposited in the standard counting gas environment. For the application in spin echo techniques (MIEZE) [3] it has furthermore been managed to extract the signal of the charge traversing the stack to identify the very thin conversion layer of about $1\mu\text{m}$. This allows to precisely determine the time-of-flight [4].

The detector concept and measurement results will be presented.

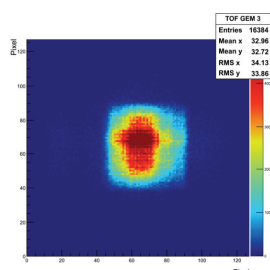


Fig. 1: Beam profile measured with 128x128 pixels at RESEDA (FRM II Munich)

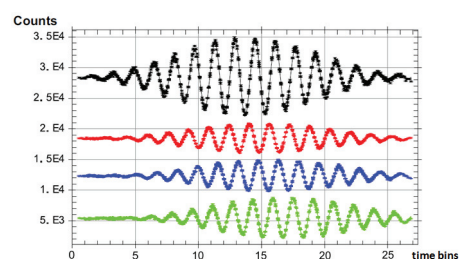


Fig. 2: Spin Echo Group of a 71 kHz MIEZE signal at different GEM foils, measured at RESEDA (FRM II Munich)

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P32

Polarizing neutron optics from Helmholtz-Zentrum Berlin

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In the last years a variety of polarizing neutron optical devices has been developed at HZB, mainly solid state elements where the neutrons are transported in thin silicon wafers with coated walls.

We show results of solid state polarizing benders, solid state collimators with polarizing walls and a solid state radial bender for the polarization analysis of neutrons over an angular range of 3.8 deg.

Another device consists of a solid state polarizing bender without absorbing layers used together with a collimator, which allows polarizing or analyzing neutrons without deflecting them from their original direction.

Two-dimensional polarization analysers for an angular range of 5 degrees in both directions are presented.

A polarizing cavity in a guide with a cross section of 60mm x 100mm was built which polarizes neutrons with wavelengths above 0.25nm.

In all these polarizing devices polarisations of 95% were realised.

Recently a polarizing S-bender with a cross section of 30mm x 100mm was tested, showing at a wavelength of 4.4Å a polarization above 98% and a transmission above 65%.

P33

MARIA – The high-intensity polarized neutron reflectometer of JCNS

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The JCNS has installed the new, high-intensity reflectometer MARIA in the neutron guide hall of the FRM II reactor in Garching. This instrument uses a velocity selector for the monochromatization of the neutron beam, an elliptically focussing guide to increase the flux at the sample position and a double-reflecting super mirror polarizer to polarize the entire cross-section of the beam delivered by the neutron guide.

Unique features of MARIA include (i) vertical focussing with an elliptic guide from 170 mm down to 10 mm at the sample position, (ii) reflectometer and GISANS mode, (iii) polarization analysis over a large 2d position sensitive detector as standard, (iv) adjustable wavelength spread from 10 to 1 % by a combination of velocity selector and chopper, (v) flexible sample table using a Hexapod for magnetic field and low temperature sample environment and (vi) in-situ sample preparation facilities. Together with a 400 x 400 mm² position sensitive detector and a time-stable ³He polarization analyser based on Spin-Exchange Optical Pumping (SEOP), the instrument is dedicated to investigate specular reflectivity and off-specular scattering from magnetic layered structures down to the monolayer regime. In addition the GISANS option can be used to investigate lateral correlations in the nm range. This option is integrated into the reflectometer's collimation, so it can be chosen during the measurement without any realignment.

MARIA is a state of the art reflectometer at a constant flux reactor. It gives you the opportunity to do easily specular reflectivity measurements in a dynamic range of up to 7-8 orders of magnitude, simultaneously with the detection of the off-specular scattering and if needed change on the fly to the GISANS configuration. Even simple SANS measurement are possible. Everything fully polarised or unpolarised. So we will discuss how MARIA can help you to investigate the depth resolved vector information of your magnetic samples.

P34

Diffraction Studies with Hot Neutrons on HEiDi

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There are two advantages from using hot neutrons for single crystal diffraction. Firstly, the extended accessibility of reciprocal space offers excellent accuracy for structural studies. Not only atomic positions and magnetic moments can be determined within small error bars but also mean square displacements that contain often valuable information about dynamic or static disorder. In addition, the different Q-dependence of the nuclear and magnetic interaction with neutrons allows to determinate both the nuclear and magnetic order very accurately within the same Bragg data set. Secondly, wavelengths below one Angstrom overcome problems generated by strong neutron absorbers like Cd, Gd, Sm, Eu in compounds.

The single crystal diffractometer HEiDi (collaboration of RWTH Aachen and JCNS) uses the hot source at the Heinz Maier-Leibnitz Forschungs-Neutronenquelle (FRM II) in Garching. The concept of this instrument focuses on flexibility and efficiency. Therefore, its spectrum of applications covers not only traditional crystallographic and mineralogical studies [1 - 4] but also contributes also to detailed investigations on potential compounds for future energy and information technology like hydrogen or ion conductors [5], HT superconductors [6] and multiferroics or other compounds with interesting electrical or magnetic features [7-9].

On the conference a brief overview of the instrument and recent instrument developments will be presented along with examples of different topics studied there.

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P35

Jalousie: a highly efficient, large area ^{10}B neutron detector **G. Modzel¹, M. Henske², M. Klein^{1,2}, M. Köhli¹, P. Lennert¹, C.J. Schmidt^{2,3}** **and U. Schmidt¹**

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The Jalousie detector is intended as a replacement for ^3He tubes, solving the ^3He availability crisis. By interposing eight tilted ^{10}B Boron layers in the neutron beam a similar efficiency is achieved. The tilting increases the effective absorption length of the ^{10}B layers, while keeping the escape length of the conversion products constant. Highly integrated readout electronics and FPGA based data analysis make a high number of channels and the resulting high data rate feasible.

The detector was designed in a modular fashion. Each lamella shaped submodule is an independent entity and consists of a two multi wire proportional chambers enclosed by ^{10}B conversion layers. By stacking these submodules, several square meters of detection area can be achieved. Since the detector operates at normal pressure and the readout electronics is placed at the back of the detector, the blind area can be minimised.

The detector is currently in prototyping stage for POWTEX at FRM II. The current spatial resolution is about 5 mm (FWHM). The detector will form a cylindrical detection area of 9 sqm, with the readout channels oriented towards the scattering center.

Concept and measurement results of the prototypes will be presented, showing that the design parameters have been achieved.

P36

Spin-Echo-Spectrometer Design for ESS

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Within the German ESS design update project [1] we are investigating optimized designs for neutron spin-echo spectrometers. First the very high resolution type was considered. The optimization was separated in two main parts: beam transport from a (cold) moderator to the sample and magnetic layout of the secondary spectrometer to enable the best resolution. Beam transport and beam polarization is obtained using a straight, 8 cm x 8 cm neutron guide with a comparatively short (~2m) polarizing bender. The bender shall have 4 channels with a $m=4$ FeSi multilayer coating. The moderator-detector distance may be chosen between 35 and 55 m. A system of 4 disc choppers to select the used wavelength frame and to suppress frame overlap is placed along the neutron guide section.

The layout of the proper (secondary) spectrometer follows a combination of design principles, which have been used in the SNS-NSE spectrometer and a strategy to find a magnetic coil configuration with minimal intrinsic field integral inhomogeneity, which was used by Farago to device new IN15 coils that shall be implemented in the 2014 break of ILL operation. By combining the active stray field compensation techniques used at the SNS-NSE, which require the use of supercomputing coils, and coil geometry optimization towards the simultaneous minimum of field-integral inhomogeneity, depolarization and stray-field a solution was found. The resulting configuration has a 3 times reduced intrinsic inhomogeneities of field integrals and low stray fields allowing for a working NSE-configuration up to 2 Tm field integral. The superconducting configuration to be realized is more challenging than the SNS-NSE configuration, however, not so complicated or bulky to be prohibitive.

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P37

Focusing mirror VSANS diffractometer KWS-3: merging nano- and micrometer worlds

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KWS-3 is a very-small-angle-neutron-scattering (VSANS) diffractometer using focusing mirror to achieve a high Q-resolution $4 \cdot 10^{-5} \text{ \AA}^{-1}$ built as a complimentary instrument aimed to fill the gap between the Bonse-Hart and pinhole cameras. A number of improvements that have been carried out during the last years and a high brilliance of the FRM-II reactor in Garching allowed for the increase in neutron flux by more than twenty times in comparison to the FRJ-2 reactor in Jülich; a further significant flux gain is expected after refurbishment the neutron guide. The Q-range of KWS-3 covers almost three decades - from $4 \cdot 10^{-5}$ to $3 \cdot 10^{-2} \text{ \AA}^{-1}$. VSANS applications can be found in different branches, like colloid science (mixtures of particles, strongly correlated colloid crystals, particles of micron size, silicon macropore arrays), materials science (filled polymers, cements, microporous media) and polymer science (constrained systems, emulsion polymerization).

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POLI: The new single crystal polarized neutron diffractometer for investigation complex magnetic structures at FRM II

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POLI is a new single crystal polarized neutron diffractometer [1] at the hot source of the 'Forschungsneutronenquelle Heinz Maier-Leibnitz' (FRM-II) in Garching, Germany. It is designed to perform spherical neutron polarimetry (SNP) in zero field as well as classical polarized neutron diffraction (PND) measurements (flipping ratio) under applied magnetic fields. Among the intended applications of this instrument are: complex magnetic structures and magneto-electric coupling in multiferroics, magnetic structure and spatially resolved spin densities in molecular magnets, magnetically ordered superconductors, strongly correlated transition metal oxides and spin chain compounds. The instrument is unique in the sense that it combines a variable wavelength focussing monochromator with the use of ^3He spin-filter cells (SFC) to create polarized, short wavelength neutrons. A new zero-field polarimeter Cryopad [2, 3] has been built in cooperation between RWTH and ILL. On the detector side, the polarisation-analysis and detection unit DECPOL (again with ^3He -spin filter cells) is used. This setup called 'POLI@HEIDI' is operational and open for users at FRM-II over JCNS proposal system. The examples of using SNP on POLI@HEiDi for the investigation on the magnetic and magneto-electric domains in different compounds (superconductors, multiferroics, quantum-phase transitions) will be presented.

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WITHDRAWN

P40

Chopper system design for the instruments at pulsed and continuous neutron sources

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Chopper systems in the TOF instruments enable us to gain control over instrument parameters which define instrument performance (resolution, pulse width, repetition rate) and allow therefore for high degree of flexibility. Considerable experience was collected in the chopper system design over the years that allows for improving the instrument performance. For instance, better focused chopper system on NEAT at HZB and upgraded IN5 at ILL resulted in substantial intensity gain at the same resolution. Further improvement can be achieved by application of the trapezoidal pulse shape and optimization of the instrument length which is implemented on NEAT upgrade project.

The operation of a major part of the instruments on the future European Spallation Source will be based on novel multiplexing techniques, such as Repetition Rate Multiplication and Wavelength Frame Multiplication (WFM). These techniques allow keeping the flexibility of the instrumental configuration and in the same time using the benefit of the ESS high peak flux. The design of chopper systems for realization of multiplexing methods differs from those at a reactor. Similarly to the reactor based instruments the main requirement for multiplexing chopper system is to assure that a neutron detected at any given time can only come from a single pulse shaping chopper pulse. However, multiplexing entails specific conditions leading to “quantized” chopper configurations in terms of the choice of the chopper positions L_i and chopper frequencies f_i relative to the source and source frequency f , respectively. The principles of the multiplexing chopper system for various applications in spectroscopy as well as in diffraction have been recently successfully tested using reactor based instruments, the TOF spectrometer NEAT at HZB, Berlin and the TOF diffractometer at BNC, Budapest, operating in non-standard modes. In these studies the pulsed source has been emulated either by a disc chopper rotating with 10-40 Hz or defined by the chopper system as a virtual pulsed source operating around 10 Hz. The results of the studies provide important input for design and operation of multiplexing instruments at ESS.

In this presentation we review our experience which we collected designing instruments for both, continuous and pulsed sources. The principles of design of the multiplexing chopper system will be demonstrated using results of our studies and a potential instrument at ESS. Further we propose a new method of multiplexing WFM that is based on the phase slewing, asynchronous operation of the pulse shaping chopper with respect to the source pulses. Using this method we can simplify and increase the speed of the data collection. It also helps to avoid systematic errors due to the overlap of individual frames and makes multiplexing WFM exactly equivalent to the common, well established TOF diffraction methods operating with a single wavelength frame.

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The upgrade of IN12

Simulations and first neutron measurements

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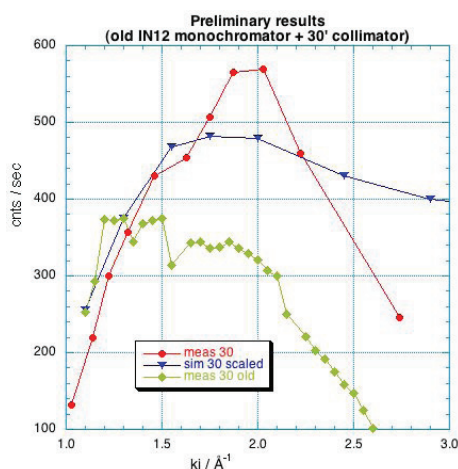
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IN12, a three-axis spectrometer for cold neutrons, is operated as a CRG-instrument from the Jülich Centre for Neutron Science (JCNS) at the Institute Laue Langevin in Grenoble. In the framework of the Millennium Program of the ILL IN12 has been relocated to a new position at the end of a new guide. Along with this relocation the whole primary spectrometer has been upgraded with new state-of-the-art components. The main improvements concern a new optimized focusing neutron guide together with a new double focusing monochromator. In addition a velocity selector has been installed for background improvement and the suppression of higher order reflections on the monochromator. For the use of polarized neutrons a new transmission polarizer (cavity) will be placed in the neutron guide, mounted on a guide changer together with a standard guide element. This guarantees high intensities and an easy change from non-polarized to polarized mode. In this presentation we will show details of the design and optimization of the various neutron optical components.

The new neutron guide has been installed recently and the first neutron tests have already been started, presently using the old vertically focusing IN12 monochromator. The new double focusing monochromator will be installed end of July 2012. This allows us to present the first flux measurements and compare them to the calculations. They also serve as a basis for an extrapolation to the final set-up with the new monochromator.

In early September 2012 we will therefore be able to show the final results for the neutron flux on the upgraded IN12 and offer the first experiments on IN12 for “friendly users”.



The figure shows preliminary measurements with our standard neutron monitor at the sample position using the old IN12 monochromator and a collimated neutron beam (30'). The active surface was reduced to 1 cm². Shown are data from the old IN12 (green) together with the new data from 6th July 2012 (red). Also plotted are the calculated count rates (blue), scaled to the data. The data show that already in this set-up the count rates are in general higher and extended to higher k_i . The change to the final set-up with the new monochromator and double focusing optics should bring an additional factor of 10 (at high k_i) to 20 (at low k_i).

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The new neutron diffractometer “BioDiff” optimized for crystals with large unit cells at the FRM II

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The diffractometer BioDiff is a joint project of the Forschungszentrum Jülich (FZJ/JCNS) and the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II). BioDiff is especially designed to collect data from crystals with large unit cells. The main field of application is the structure analysis of proteins, especially the determination of hydrogen atom positions. A highly orientated pyrolytic graphite monochromator (PG002) allows to operate BioDiff in the wavelength range of 2.4 Å to about 5.6 Å. A neutron velocity selector removes higher order wavelengths contaminations. To cover a large solid angle the main detector of BioDiff consists of a neutron imaging plate system in a cylindrical geometry. A Li/ZnS scintillator imaged onto a CCD-chip is available for additional detection purposes (see Fig. 1, left). BioDiff is equipped with a standard Oxford Cryosystem “Cryostream 700 plus” which allows measurements in the temperature regime from 90 K up to 500 K. The main advantage of this instrument is the possibility to adapt the wavelength to the size of the unit cell of the sample crystal. Applications of the BioDiff instrument as a powder diffractometer are also discussed.

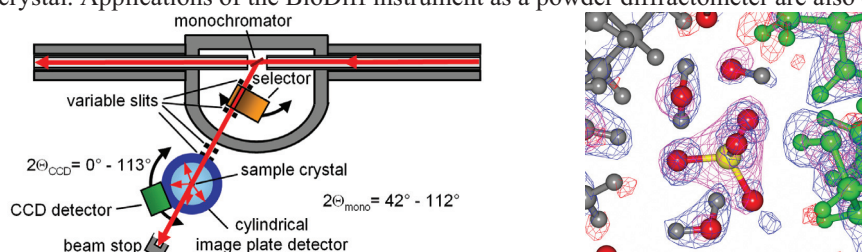


Figure 1 Schematic view of the instrument BioDiff (left). A first neutron map recorded on a myoglobin crystal is shown on the right. The x-ray map is shown in magenta at a contour level of $+2.7 \sigma$. The nuclear map is shown at a contour level of -1.75σ in red and at $+2.3 \sigma$ in blue. The water network (and a sulfate ion) in this contact region between two myoglobin molecules is nicely seen.

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Neutron energy analysis by silicon prisms

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Neutron energy analysing techniques are of great interest, because they provide the possibility to measure at different wavelengths at the same time. This is a big advantage compared to crystal monochromators where only one certain wavelength is available. Chopper systems used in time-of-flight mode provide high resolution but low transmission compared to the intensity of the white neutron beam. With a refractive energy analysing device the intensity of the beam is only reduced by the attenuation in the material. We present an energy analyser consisting of silicon prism layers. These layers are produced with an anisotropic etch process and can be stacked upon each other without producing any additional material in the beam. We measured at the EROS reflectometer at the LLB and refracted a $25 \times 0.3 \text{ mm}^2$ beam with 191 silicon prisms and could achieve a wavelength resolution of 5% at 6.7 \AA in a distance of 2 m to the detector.

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Bispectral powder diffraction at the long pulse source ESS

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Within the ESS design update programme, funded by the German Federal Ministry of Education and Research, we investigate a versatile instrument concept for powder diffraction at the ESS. Typical applications will be the determination of structures involving light elements, complex magnetic structures, and the ability to follow phase transitions in reactive materials or in functional materials *in-situ* under conditions close to operation. To match the various needs, we propose a bispectral [1,2] time-of-flight diffractometer efficiently using thermal and cold neutrons. A wide wavelength spectrum is of interest to exploit the backscattering option with high resolution. Choosing a wavelength band of 0.8 to 4.6 Å, for the given repetition rate of 14 Hz of the ESS source, the time-of-flight frame will be filled for a 75 m long instrument. The chopper system of counter rotating discs at a minimal distance of 6 m from the moderator will provide a flexible resolution from 10 µs to 1 ms for two sub-pulses for thermal and cold neutrons. The aperture of the chopper system at 6 m from the moderator defines an image of 5 to 10 mm diameter with an initial divergence of $\pm 0.6^\circ$. The desired phase space density that can be transported by elliptic guides to the sample position of similar size, with only small losses, by current neutron guide qualities as shown by our VITESS Monte Carlo simulations, which use a recently developed back-tracing algorithm [3]. Moreover, the chopper's aperture represents an important eye-of-the-needle for reducing background by more than two orders of magnitude and will also help to design more cost-efficient shielding. While the final detector choice may depend on many currently ongoing developments, it is clear that there will be a request for large solid-angle coverage with a high spatial resolution adapted to typical small sample sizes.

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Capabilities and science highlights on the ISIS second target station reflectometers

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Seven new instruments for neutron scattering have been built at the ISIS second target station providing new opportunities in surface science, disordered materials, magnetic diffraction, small-angle neutron scattering and slow dynamics. Neutron reflectometry is a powerful technique for studying surfaces and interfaces between solids, liquids and gasses, and three state of the art reflectometers are presented. Inter builds upon the success of the world-leading Surf instrument at ISIS and provides a unique facility for the study of air/liquid, liquid/liquid, air/solid and liquid/solid interfaces. Offspec characterises the increasingly important area of in-plane interface structure using the spin-echo technique. Through delicate manipulation of polarised neutrons, small structures with sizes from 10-1000 nm can be examined in thin-film samples. Polref is a polarised neutron reflectometer designed for the study of the magnetic ordering in and between the layers and surfaces of thin film materials. Three-directional polarisation control allows unique information to be obtained on the size and direction of the magnetism as a function of depth in multi-layer structures. Scientific highlights from each reflectometer will be presented. In addition, an overview over the phase two spin-echo reflectometer “Larmor” will be given.

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DNS – A versatile diffuse neutron scattering spectrometer with polarization analysis at FRM II

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DNS is a versatile diffuse scattering instrument with polarization analysis operated at FRM II. With its compact design, large double-focusing monochromator and highly efficient supermirror based polarizer, DNS offers an impressive polarized neutron flux in the range of 10^7 n/(cm²s). DNS has become very attractive for the studies of highly frustrated spin systems [1], strongly correlated electrons [2], emergent functional materials [3] and soft condensed matter [4]. With the combination of large-array position sensitive detectors covering 1.9 sr of solid angle and a high-frequency disc chopper system, both under development, DNS is expected to become a high count-rate cold time-of-flight spectrometer with medium resolution. The current status and ongoing instrument developments as well as recent scientific highlights at DNS will be presented in details.

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E9 after the upgrade: performance and abilities

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The fine-resolution neutron powder diffractometer E9 at the BER II reactor at the Helmholtz-Zentrum Berlin für Materialien und Energie [1] has undergone major alterations, which improved both the performance and the flexibility of the instrument. The layout between source and sample remained unchanged [2], with the monochromator - reactor core distance of 11 m allowing a large take-off angle, reduced number of epithermal neutrons in the primary beam from a sapphire single crystal filter, and a vertically focussing Ge-monochromator of 300 mm height allowing flexible optimization of the focus of the secondary beam. The original 64 channel linear wire detector (old D2B type) [2] has been replaced by a detector consisting of eight individual 2D detectors with 300 x 300 mm active area and a radial collimator to reduce background noise. The individual detectors are arranged at an optimized, non-constant distance from the sample. With this novel setup, complete diffraction patterns of the whole diffraction range are now accumulated in only three steps. Position-sensitive data integration results in a strongly reduced asymmetry of the peaks. Through the choice of sample diameter, axial focus length, and primary collimation a wide range of combinations of intensities, resolution curves and sample volume can be obtained. In example, the resolution of the original E9 can be matched with increased intensity from a smaller sample volume. If a slightly relaxed resolution is accepted, much higher intensities can be achieved. In this mode, the instrument is dedicated to collect diffractograms suited for crystal structure determinations and Rietveld refinements with unit cell volumes up to 1000 Å³. This is equivalent to the original dedication, but with increased data collection speed. Additionally, four of the individual detectors can be placed at variable distances from the sample, in a new high intensity conformation of the instrument. This mode is suitable for atomic and magnetic structures with small unit cells and high symmetry, and also for particularly small samples. In this configuration each individual detector covers a large angular range. This is useful for data collection with fixed detector position, allowing for rapid parameterized scans, e.g. temperature or field strength dependency of magnetic structures, cavity fillings or phase compositions. Combining different distance selections is possible, e.g. to measure magnetic diffraction peaks at low angles with high intensity, while simultaneously measuring peak shifts from magnetostriction with high resolution at high diffraction angles. The 2D-data are directly accessible, e.g. to perform texture analysis. Of course, the upgraded instrument still allows the use of the usual suit of sample environments, covering a wide range of low and high temperatures, pressure, variable magnetic fields, and controlled gas atmosphere. With BER II back in operation, E9 is now once again open to applications [1] from external users.

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Development of a multi-band direct geometry chopper spectrometer for the future European Spallation Source

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Within the ESS Design Update Phase Programme funded by the German Federal ministry of education and research, we investigate the performance of a set of spectrometer concepts at the long pulse source of the ESS, which promises the applicability to a wide manifold of scientific activities of research: strongly correlated electron materials, disordered systems, functional materials, magnetism, soft-matter and biophysics. Here we present the current state-of-the-art in the study of the multi-band instrument concept and describe the main aspects of the conceptual design.

The useful beam at the sample position is an important figure of merit in the evaluation of the instrument performance and can represent a limit to possible scientific applications in several circumstances, when high flux is requested. Thus the problem of the beam transport to the sample is under careful consideration, in order to transport as much as possible of the phase space density provided by the source, while maintaining as low as possible the back-ground contamination coming from the direct view of the moderator surface.

The chopper system is a crucial aspect in order to achieve useful resolution for a manifold of scientific purposes. The aim is to make an efficient use of the flux provided by the source, by means of the Repetition Rate Multiplication (RRM), while reducing contamination due to very fast and very slow neutrons. We present the chopper layout under investigation and the method for the RRM implementation, based on the commensurate choppers technique.

The necessary requirements for the detector development in terms of spatial and time resolution are already evaluated and the implications deriving from technical limitations on this task are discussed.

Preliminary results of virtual experiments performed by means of beam neutron ray-tracing simulation packages are presented, in order to show the estimated performances, especially focusing on the resolution function evaluation.

Finally we discuss the implications in the use of the polarization analysis for a large bandwidth instrument.

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Progress report on the novel time-of-flight spectrometer with polarization analysis TOPAS

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We report on the progress of the construction of the new thermal time-of-flight spectrometer TOPAS, being installed at the FRM II. The spectrometer features a high monochromatic flux in the energy range $20 \text{ meV} < E_i < 150 \text{ meV}$, provided by an elliptic neutron guide and a chopper system comprised of 2 Fermi choppers to define the energy resolution and a disc chopper for contamination removal. The most prominent feature of the instrument is the polarization option. The incident beam is polarized by a compact continuously pumped SEOP polarizer, developed at JCNS for SANS applications. The ^3He polarization achieved is as high as 80 %. For the polarization analysis we develop a wide angle ^3He spin filter cell and coil arrangement with large solid angle coverage and minimized blind spots.

In the poster we present the progress in the construction of all components of spectrometer, which will be installed at the FRM II in the new eastern neutron guide hall.

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Standard, advanced and complementary sample environment at the Helmholtz-Centre Berlin

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Important for the successful operation of a neutron or x-ray facility is certainly to provide the scientific users the best technical and scientific support to perform highest impact experiments. Beside other technical, scientific or administrative tools and services, the quality of the available sample environment support is a key aspect for excellent scientific results. This poster contribution will show up, how sample environment department at the Helmholtz-Centre in Berlin is involved in the realization of distinguished neutron scattering research.

The unique material penetrating property of neutrons allow investigations under extreme environment conditions with respect to highest and lowest temperatures, magnetic- and electric fields, mechanical pressure and gas atmospheres. The sample surrounding equipment to implement these conditions and combinations of them in a neutron scattering experiment are provided almost as standard sample environment tools at the neutron facility in Berlin.

Due to the general trend to combine also neutron scattering with complementary in-situ investigation methods like IR-spectroscopy and rheometry or susceptibility measurements, as well as the increasing number of experiments with in-situ sample preparation by physical and chemical means, more advanced sample environment equipment is available on site. Such equipment is in many cases dedicated to special scientific topics and scattering methods (i.e. small angle scattering and reflectometry) and has been developed from the scientific- or instrument responsables in cooperation with sample environment experts.

Finally, the HZB supports the neutron and photon user communities beyond their particular beamline investigation by offering different sample preparation and characterization. Two of them, the GasLab (DEGAS) and MagLab (LaMMB), are operated from the sample environment department, profiting thereby from the available expertise and equipment, which allows also non standard complementary ex-situ investigations.

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EPSILON-MDS - The German high resolution TOF diffractometer at the pulsed neutron source IBR-2M

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The long pulsed neutron source IBR-2M, which works with a pulse frequency of 5Hz and a long pulse length of 320 μ s for thermal neutrons, has been upgraded in the last years and put into operation in 2012 [1]. The KIT Karlsruhe operates the high resolution ($\Delta d/d = 4 \cdot 10^{-3}$) time-of-flight multi-detector diffractometer EPSILON-MDS as a strain/stress diffractometer with a 4-axis goniometer. The instrument is characterized by a long flight path of about 105 m and the available wide wavelength range up to $\lambda_{\max} = 7.1$ Å. The new Ni-covered neutron guide is constructed as a bent neutron guide ($m=1$) with a radius of curvature of 13 400. Using an additional beam-chopper the wavelength can be expanded up to $\lambda_{\max} = 12$ Å, so low indexed peaks with d -ranges up to 8.5 Å can be investigated [2].

The diffractometer EPSILON-MDS as a time-of-flight diffractometer with its technical parameters has no analogue in Germany. The main features of the instrument are a $2\theta=90^\circ$ geometry, nine detector banks, each of them are equipped by nine ^3He detectors.

This diffractometer is equipped with an uniaxial pressure device up to 100 kN, to carry out deformation experiments at samples of $d = 30$ mm, $l = 60$ mm with pressures up to 150 MPa and allows a sample rotation under load [3], an acoustic emission detection system for the detection of micro-cracks and a laser extensometer for measurements of macro-stresses of the sample. Furthermore, a Paris-Edinburgh-cell (VX4) allows the deformation of small samples with pressures up to 8 GPa.

With the described parameters and the sample environment the instrument can be used for a wide range application, but preferential for the investigation of polycrystalline samples with lower crystal symmetry, as they occur in mineralogical samples, but also for other materials, like ceramics can be investigated. The diffractometer EPSILON-MDS is now at the disposal of the interested community.

The high neutron flux and high resolution achievable with TOF technique allow already today to perform and optimize at EPSILON-MDS experiments which are planned for ESS.

This project is supported by the German Ministry of Education and Research.

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The new neutron guides at the 7th beamline of the fast pulsed reactor IBR-2M in Dubna

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The shut-down of the fast pulsed reactor IBR-2 at JINR Dubna has been used to renew the neutron guide for the EPSILON¹⁾ and SKAT diffractometers at the 7th beamline.

The 7th beamline serves two diffractometers (EPSILON and SKAT) and a spectrometer (NERA) with pulsed neutrons. All three facilities are located in a pavilion at a distance of more than 100 m from the surface of the moderator. Up to now the moderator is a “grooved” light water moderator at ambient temperature. But in the future this beamline partly “sees” a cold solid mesitylene source at a temperature of about 20 K.

In order to decrease the neutron and the γ -ray background the neutron guides are bent with a radius of curvature of 13 400 m, while the guide for the spectrometer is a straight one. The cross section of the bent guides is $50 \times 95 \text{ mm}^2$ (width \times height).

To prevent the pollution of the beam with delayed neutrons and γ -rays at a distance of 5.5 m from the moderator there is a disk chopper rotating synchronously with the moveable reflectors of the reactor. The disk has an opening of 60°. Directly after the background chopper is situated a beam splitter for dividing the beam into the three beams. The length of the splitter is about 10 m and at the end of the splitter starts the bent part of the guides for EPSILON and SKAT. The length of the bent parts is about 85 m, followed by another straight part in order to homogenise the neutron beam.

At a distance of about 20 m there are additional drum choppers. The chopper may rotate with the half of the velocity of the background chopper and may therefore suppress every second power pulse. By this simple mean one can extent the wavelength band of the incident beam up to 12 Å. In the case when the additional chopper is switched off the wavelength is limited to 7.4 Å due to frame overlapping.

The high neutron flux and high resolution in TOF geometry allow already today to perform and optimize at EPSILON-MDS many experiments which are planned for ESS.

This project is supported by the BMBF.

¹⁾ See F.R. Schilling *et al.* “EPSILON-MDS – the German ...”, this conference

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The E3 Residual Stress Neutron Diffractometer Upgrade

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Since 2011 the Residual Stress diffractometer E3 has been in the process of an upgrade. The newly installed electronics enable future options to be implemented making more efficient use of neutron beamtime by making the instrument more automated and easier to use. One future option will be a fully automated primary slit system enabling easy and precise change of the primary neutron beam optics without time consuming adjustment. This will be part of the planned fast alignment and set-up procedure, increasing the available measurement time and together with a new Eulerian cradle, the measurement of strain in three orthogonal directions in one fully programmable configuration is the goal.

Since the reactor start-up in 2012 a number of measurements have been performed. A selection of these showing the strengths of E3 will be presented.

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The high resolution neutron backscattering spectrometer SPHERES

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The SPectrometer for High Energy RESolution (SPHERES) is a third generation neutron backscattering spectrometer with focusing optics and a phase space transform chopper. It provides high energy resolution ($\sim 0.65 \mu\text{eV}$) with a very good signal-to-noise ratio [1]. By filling the instrument housing with argon in order to avoid air scattering in the secondary spectrometer the signal-to-noise ratio has been increased by about 50%. A further gain in flux will be achieved by a more efficient phase space transform chopper which is currently under development. SPHERES is a versatile spectrometer for investigating atomic and molecular dynamics on a GHz scale. Typical applications include hyperfine splitting in magnetic materials, molecular rotations, diffusion and relaxation processes in various systems.

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P55

Magnetization reversal in Nd-Fe-B based nanocomposites as seen by magnetic neutron scattering

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We have investigated the magnetization-reversal process in a Nd₂Fe₁₄B/Fe₃B nanocomposite by means of magnetic-field-dependent small-angle neutron scattering (SANS). Based on the computation of the correlation function of the spin misalignment we have estimated the characteristic size l_C of spin inhomogeneities around the hard magnetic single-domain Nd₂Fe₁₄B nanoparticles. The quantity l_C approaches a constant value of about 12.5nm (close to the average particle radius) at 14T and takes on a maximum value of about 18nm at the experimental coercive field of $\mu_0 H_c = -0.55$ T. The field dependence of l_C can be described by a model that takes into account the convolution relationship between the nuclear and magnetic microstructure.

P56

Uniaxial pressure studies of helimagnetic order and the skyrmion lattice phase in MnSi

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We report small angle neutron scattering and ac susceptibility measurements of the uniaxial pressure dependence of the helimagnetic order and the skyrmion lattice phase in MnSi. For our studies a bespoke sample stick with a He-activated bellow system has been built that permits simultaneous neutron scattering and susceptibility measurements. We find that both the helimagnetic order as well as the skyrmion lattice phase are very sensitive to the application of uniaxial stress. Besides a reorientation of the skyrmion lattice the most prominent effect is either a pronounced suppression or an enhancement of the skyrmion lattice phase depending on the field and stress direction. We discuss our results in the context of the mechanism that stabilizes the skyrmion lattice phase.

P57

Exchange interaction in $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ multilayers

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The ternary alloy $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ exhibits a rich magnetic phase diagram with ferromagnetic (FM) and antiferromagnetic (AF) phases in dependence on the Rh concentration and temperature [1]. Studies on films with a thickness of about 200nm thickness allowed us not only to identify the different magnetic states in dependence on the Rh concentration and temperature, but also to get access to the different spin configuration accompanied with the magnetic ordering (see Fig. 1) [2]. For low Rh concentration of $x < 10$, a FM phase with a dominant in-plane ordering was found while the films with $x > 10$ exhibit an AF phase with a dominant out-of-plane ordering. Particularly films with an Rh concentration of about 10% are interesting since they exhibit an AF-FM transition which qualifies these systems for future technological applications such as magnetic underlayers or magnetic sensors.

The interplay between $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ films with different Rh concentrations were investigated using polarized neutron reflectometry and SQUID. We investigated multilayers consisting of 8 bilayers grown on Al_2O_3 (11-20) substrate to introduce in-plane anisotropy for the FM components if present of different concentrations as the following:

$\text{Fe}_{50}\text{Pt}_{45}\text{Rh}_5(10\text{nm})/\text{Fe}_{50}\text{Pt}_{32.5}\text{Rh}_{17.5}(20\text{nm})$ (SampleA), $\text{Fe}_{50}\text{Pt}_{40}\text{Rh}_{10}(10\text{nm})/\text{Fe}_{50}\text{Pt}_{32.5}\text{Rh}_{17.5}(20\text{nm})$ (SampleB).

Using the polarized neutron reflectometry, we obtained the depth resolved magnetic profiles of exchange coupled $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ (FPR_x) multilayers. An induced in-plane magnetization was observed throughout the AF layer. After cooling to 90K in a magnetic field of 1 T a significant exchange bias effect could only be observed in the out-of-plane direction instead of the in-plane direction as expected if the exchange bias effect is due to the exchange between the interfaces of the different concentrations (see SQUID measurements in Fig2). The result indicates strongly that the out of plane exchange bias originates from the FPR₁₀ layer itself, which exhibits both the AF and FM phases as it observed in the bulk material as well as thick films.

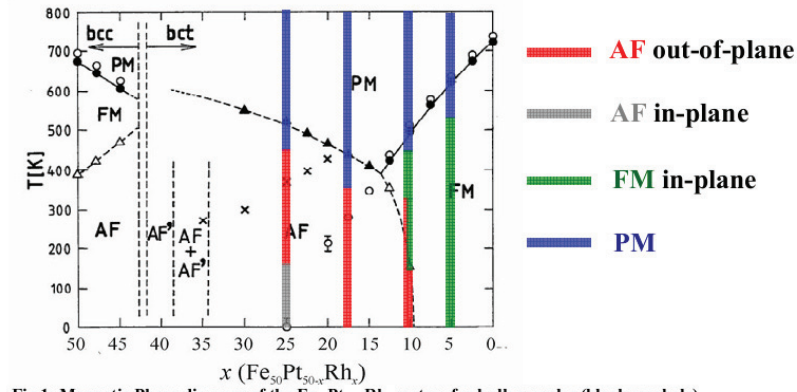


Fig.1: Magnetic Phase diagram of the $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ system for bulk samples (black symbols) [1] and 200nm thin films (coloured bars).

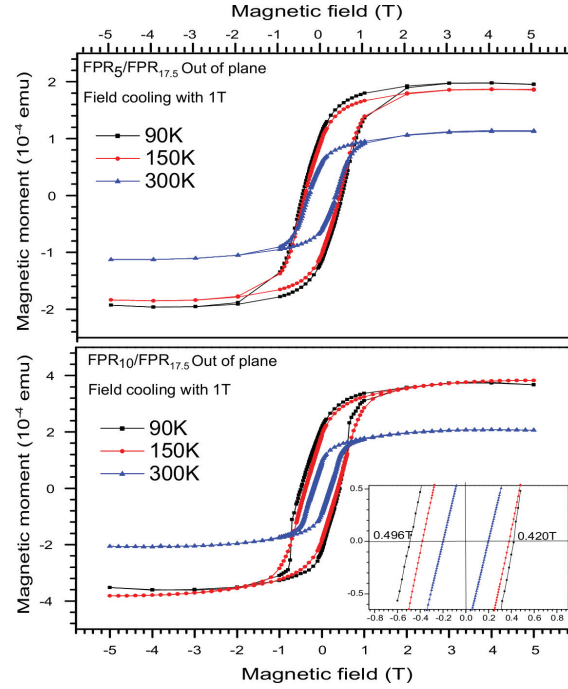


Fig2. SQUID measurement in the out of plane direction after 1T field cooling of FPR₅/FPR_{17.5} (up) and FPR₁₀/FPR_{17.5} (down). A significant exchange bias up to (38 mT) was observed in the out of plane direction in FPR₁₀/FPR_{17.5} at 90K and no exchange bias in FPR₅/FPR_{17.5}.

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P58

Origin of exchange bias in DyCo/FeNi system

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The exchange interaction between a magnetically soft and hard layer is of great interest, in particular in thin films and multilayer systems that play an important role for many spintronic devices [1]. This so called exchange bias effect is in general caused by the uncompensated spin configuration at the interface resulting in a significant increase of the coercivity. However, besides the classical FM/AF system the exchange bias effect can be also observed in systems where the AF as hard magnetic layer is replaced e.g. by a magnetically hard ferromagnetic material. A very interesting system in this respect is the DyCo/FeNi bilayer structure in which the permalloy layer serves as the magnetically soft FM layer with an in-plane anisotropy while the magnetically harder ferrimagnetic layer DyCo possesses perpendicular anisotropy [2, 3]. The exchange bias effects can be achieved here by magnetizing the DyCo in perpendicular direction in respect to the film plane. The in-plane hysteresis of the permalloy layer shifts in dependence of direction of the pre-magnetization of the DyCo layer in the one or other direction showing a large exchange bias effect. Particularly interesting is that no increase in the coercive field is observed indicating that the effect has a different origin as for the classical AF/FM systems (as shown in Fig1). In order to shed light into the understanding of the origin of the exchange coupling, PNR can help to distinguish between two possible scenarios: the existence of multi- domains of perpendicular and parallel oriented magnetization along the sample plane in the DyCo layers and a uniform twist from the perpendicular to the parallel orientation towards the interface.

In our experiments a DyCo(79nm)/FeNi(19nm) bilayer was investigated by polarized neutron reflectivity probing the different magnetic states at both magnetization reversals at saturation as well as the remnant field. As expected only one of the magnetization branch (here called the negative branch) shows significant differences in the polarization channels for saturated (marked as B in Fig2) and low magnetic fields (marked as A in Fig2) due to the strongly shifted hysteresis loop of the magnetization curve. The simulation of the polarized neutron spectra enabled us to extract the magnetization profile of the system to identify the possible coupling mechanism in this system at the magnetic state marked as A, B, C and D, as shown in Figure 2. Figure 3 shows the according magnetization profiles for the different polarization states and magnetic fields.

Besides the expected splitting in the scattering length densities of both polarization channels for the NiFe layer at saturation a clear in-plane magnetic contribution is found across the whole DyCo layer. These findings may be interpreted that throughout the whole DyCo layer domains are present which are not only perpendicularly but also longitudinally magnetized. However, the simulation also shows a smeared out transition area in the magnetization profile of the FeNi layer towards the DyCo layer. This could be caused by twisted moments in the permalloy layer away from the longitudinal direction or possible magnetically dead domains and may have a big impact on the presence of the observed exchange bias effect.

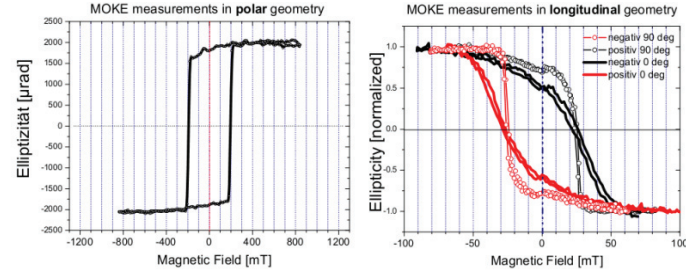


Fig.1:(left) MOKE measurement in the polar geometry of a DyCo(79nm)/FeNi(19nm) bilayer system probing the perpendicular anisotropy of the DyCo layer. (right) MOKE measurement in the longitudinal geometry of a DyCo(79nm)/FeNi(19nm) bilayer system probing the in-plane anisotropy of the FeNi layer independence of the magnetization of the DyCo layer (negative/positive = perpendicular in one or the other direction in respect to the sample plane) and the in-plane orientation (0/90 deg = two perpendicular in-plane orientation along the sample edges).

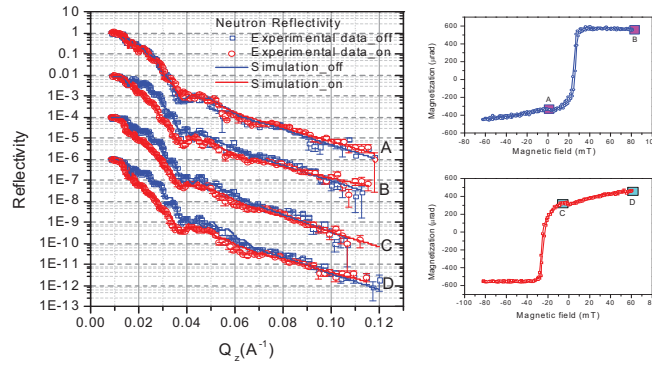


Fig2: (left) PNR results with simulation DyCo/NiFe at different states marked A, B, C and D and (right) the details of A, B, C and D from the MOKE hysteresis loops. PNR data show obvious difference in the states of A and B and slight difference in the states of C and D due to the positive and negative H_{EB} , respectively.

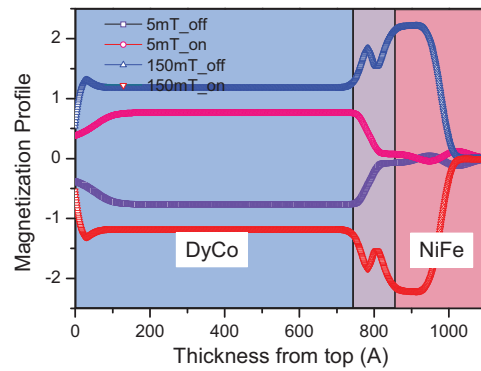


Fig3: Magnetization profiles of DyCo/NiFe bilayer with an in plane extern field of 150mT (state B) and 5mT (state A), after 1T perpendicular magnetization. Magnetization profiles for state C and D are not shown here since they are similar to state B, as shown of the almost equivalent PNR data in Fig.2.

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Magnetization reversal in laterally patterned thin films via ac-polarized neutron reflectometry

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Switching times and switching mechanisms of magnetization reversal in micro- and nanostructures have recently gained much scientific and technological interest. New intriguing ideas in spintronics such as the “Racetrack Memory” concept for ultrahigh density information storage [1] have launched numerous investigations of the domain wall kinetics in laterally confined media. Of particular interest is an understanding of the drastic change of domain wall velocity for low and high magnetic fields and the transition region in between, characterized by turbulent motion (Walker limit) [2]. Magneto-optical Kerr effect (MOKE) [3], giant magneto-resistance (GMR) [4], and x-ray photoemission electron microscopy (XPEEM) [5] have been used for the detection of domain wall propagation. In spite of common consideration of PNR as a tool for measurements in static external magnetic field, it also can be performed in the frequency domain while averaging over spatial areas corresponding to the coherence length of the neutrons. In the static case PNR detects the magnetization direction in the sample. At very high frequencies beyond a critical limit, the domains no longer can follow the external field reversal and the magnetization appears again static. Between these limits, PNR is highly sensitive to the frequency response of the magnetization reversal. For these investigations the SuperADAM reflectometer (ILL, Grenoble) has been furnished with a sample environment that allows to apply magnetic field frequencies up to 2 MHz with field amplitudes up to 120 Oe [6,7]. We will discuss recent results gained on the frequency dependence of the magnetization reversal in Py ($\text{Fe}_{0.19}\text{Ni}_{0.81}$) thin films after patterning them by lithographic means into a lateral array of microstrips.

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P60

Magnetic properties of $\text{Yb}(\text{Rh}_{0.42}\text{Co}_{0.58})_2\text{Si}_2$

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The heavy-fermion compound YbRh_2Si_2 is a model system to study quantum criticality. However, because of its very low ordering temperature $T_N \approx 70$ mK and the small size of the ordered magnetic moment μ_{AF} , the magnetic structure of YbRh_2Si_2 is still unknown. Isoelectronic doping with Co leads to an increase of T_N and of μ_{AF} [1]. Nevertheless the $(x - T)$ - phase diagram shows a marked dip near a Co concentration of 50 %, possibly associated with a change of the magnetic structure. For $x > 0.58$ the magnetic structure is incommensurate below T_N with a propagation vector $\tau_1 = (0.25 \ 0.08 \ 1)$ followed by a change to a commensurate structure with $\tau_2 = (0.25 \ 0.25 \ 1)$ at a lower temperature $T_L < T_N$. For $x = 0.58$ only the commensurate magnetic order has been found below $T_N \approx 700$ mK so far. For lower Co concentrations the magnetic structure is still unknown. To study the change of magnetic structure in more detail, we performed heat capacity, resistivity and magnetisation measurements on $\text{Yb}(\text{Rh}_{0.42}\text{Co}_{0.58})_2\text{Si}_2$, which is located near the minimum of the ordering temperature in the $(x - T)$ - phase diagram. Measurements of the heat capacity and resistivity in zero field revealed one broadened phase transition at an ordering temperature of $T_m \approx 820$ mK in contradiction to the absence of magnetic intensity in neutron diffraction experiments at the commensurate position $\tau = (0.25 \ 0.25 \ 1)$ above $T \approx 700$ mK. Magnetisation measurements lead to a first step towards a clarification of this discrepancy. We observed a first transition at $T \approx 820$ mK to a likely ferromagnetic state followed by a second transition at $T \approx 650$ mK towards an antiferromagnetic state at low fields. Recent neutron diffraction experiments in applied magnetic field $B \parallel [110]$ could confirm the magnetisation measurements, but microscopic evidence for a ferromagnetic nature of the second phase for temperatures $700 \text{ mK} < T < T_m$ is still missing.

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Observation of cross-shaped anisotropy in spin-resolved small-angle neutron scattering

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We report the results of spin-resolved small-angle neutron scattering (SANS) experiments on the two-phase nanocrystalline alloy NANOPERM. At a saturating applied magnetic field of 1.27 T we observe a cross-shaped angular anisotropy in the non-spin-flip SANS cross section Σ^{++} . This feature—for this class of materials only visible at saturation in Σ^{++} —is attributed to the specific ratio of nuclear to magnetic scattering being smaller than unity.

Analysis of the non-spin-flip and spin-flip cross sections provides the nuclear and magnetic SANS and allows us to estimate the magnitude of the respective scattering-length density contrast at the interphase between the nanoparticles and the amorphous magnetic matrix.

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P62

Strong coupling of Sm and Fe magnetism in SmFeAsO

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The magnetic structures adopted by the Fe and Sm sublattices in SmFeAsO have been investigated using element-specific x-ray resonant, nonresonant and neutron magnetic scattering techniques. Between 110 and 5 K, the Sm and Fe moments are aligned along the c and a directions, respectively, according to the same magnetic representation and the same propagation vector $(1\ 0\ 1)$. Below 5 K, the Sm moments reorder in a magnetic unit cell equal to the chemical unit cell. Modeling of the temperature dependence for the Sm sublattice provides clear evidence of a surprisingly strong coupling between the two sublattices, and indicates the need to include anisotropic exchange interactions in models of SmFeAsO and related compounds.

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P63

Resonant mode in the rare-earth-based strongly correlated semiconductors

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An extended study of the spin dynamics in the strongly correlated semiconductors YbB₁₂ [1] and SmB₆ [2] as well as in the series of related electron-doped systems [3-5 and references therein] has been performed by means of inelastic neutron scattering spectroscopy. It was found that rare-earth compounds with valence instability may demonstrate an exciton-like in-gap excitation, generally similar to the so-called *resonant mode* (RM) initially discovered in HTSC. The resonant excitations observed can be classified into two types: (1) spin-exciton-like excitations arising from dynamical antiferromagnetic correlations between the localized magnetic moments of the rare-earth ions (YbB₁₂-based systems); (2) excitations based on a charge exciton with intermediate radius in compounds with “strong” intermediate valence (SmB₆-based systems). The possible role of interplay with lattice degrees of freedom [6] is also discussed.

The results of the present study along with the literature data on the number of high-T_c, heavy-fermion- and pnictide superconductors and some magnetic compounds, point to such type of resonant excitations being characteristic for the systems with gap-like dynamical response in the presence of *competing interactions*. The analysis of RM behavior in different compounds reveals the unambiguous correlation between the character of the temperature evolution of the gap in the excitation spectrum, and the temperature dependence of RM energy. Typically on suppression of the gapped state with *increase* of the temperature the RM energy gradually decays, like the order parameter at the phase transition. However, in some systems RM energy appears to be nearly temperature-independent in the whole temperature range where RM exists, indicating the specific mechanism of the gap opening.

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P64

Polarized neutron scattering on TbNi₅ single crystal

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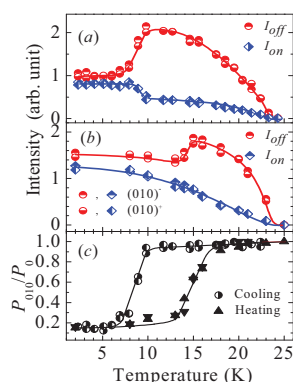
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The TbNi₅ intermetallic compound has been extensively studied by means of several experimental techniques; results of those experiments appeared to be in good agreement with a simple model of a ferromagnetic structure, which undergoes ferro-paramagnetic phase transition at $T_p = 23$ K. However, recently AC susceptibility and magnetization data indicated that the magnetic state of the TbNi₅ might well be more complex than a simple ferromagnetic structure originally thought.

In order to resolve the continuing controversy on the magnetic state of the TbNi₅, we have carried out a polarized neutron diffraction experiment.

We have performed polarized neutron diffraction on TbNi₅ single crystal by means of the triple-axis E1 spectrometer with polarization analysis at Helmholtz Centre Berlin for Materials and Energy. The product of the scattering vector and the polarization of an incident neutron beam always was equal to $\mathbf{Q} \cdot \mathbf{P}_0 = 0$.



Figs. 1a and 1b show thermal variations of intensities of the (010)[±] satellites measured at a flipper off (I_{off}) and flipper on (I_{on}) for both cooling (Fig. 1a) and heating (Fig. 1b) procedures. As one can see, there exists a distinct hysteresis with a width of about 6 K between the cooling and warming curves.

Fig. 1c presents the temperature dependency of the polarisation of neutrons, obtained for both cooling and heating curves. Both dependencies exhibit a distinctly abrupt change over a narrow temperature interval. This change occurs between 8 and 10 K for the cooling curve and from 13 to 16 K for the heating curve, respectively with the overall hysteresis of about 6 K.

We explain abrupt temperature variations of the I_{off} and I_{on} intensities for satellites over interval (10 – 8) K is related with a depolarization of neutron beam, passed through the crystal with magnetic heterogeneities. Our experimental results allow assuming that the ferromagnetic and modulated components of the Tb-ion magnetic moment are oriented in the same direction at all temperatures.

The research was partly supported by project of RFBR No. 10 – 02 – 155.

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AC-polarized neutron reflectometry of Co/Cu/Py spin valves

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Spin valve systems based on metallic ferromagnet (F) and normal metal (N) films remains to be a subject of intensive experimental and theoretical studies, although they are already widely used in various information storage and other electronic devices. One of the basic phenomena exploited in these systems is the giant magnetoresistance (GMR) effect revealed by two F layers sandwiching a thin layer of the normal metal. The electric resistivity of the trilayer strongly depends on the relative orientation of both magnetization directions in the F layers. It has recently been shown that the value of magnetization relaxation rate in F1/N/F2 spin valves with soft ferromagnetic layers can be controlled by adjusting the relative magnetization direction of F1 and F2 layers from the parallel (P) to the antiparallel (AP) state [1,2]. Dominating mechanism responsible for this effect can either be the spin-pumping induced damping effect [1,2] or the domain-wall (DW) induced coupling effect [3].

Using the ac-polarized neutron reflectometry (AC PNR) option, recently established at the Super ADAM instrument (ILL, Grenoble) [4,5], we have studied the magnetic response of the Py layer in a Co(10 nm)/Cu(15 nm)/Py(20 nm) trilayer on an AC magnetic field excitation with the direction of the *rf* field amplitude perpendicular to the direction of magnetization within the film plane. The AC frequencies (120 kHz and 1200 kHz) are kept well below the resonance frequency of the magnetic layers (GHz). This non-resonant excitation mode allows us to investigate the “magnetic stiffness (MS)” of ferromagnetic layers in the transverse AC fields. We have found that in the P configuration the magnetization of the Py layer responds more easily to changes of the amplitude and frequency of the AC field than in the AP configuration. From this we infer an enhancement of the “MS” in a transverse AC field when changing the relative orientation of the Py layer from P to AP orientation. We suppose that inversion of magnetization direction of the Py layer from P state in saturation to AP (in respect to Co magnetization) leads to induction of DW coupling between F layers by magnetostatic stray fields [3]. This may cause an enhancement of “MS” in the Py layer for a transverse AC field.

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P66

Spin structure of Fe- and Co-substituted MnSi and MnGe

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The intriguing magnetic and transport properties of the transition metal-monosilicides TM-Si (TM = Mn, Fe, Co) have been studied extensively during the last thirty years, whereas the properties of the TM-monogermanides are much less investigated due to the complexity of the synthesis. Both systems order in a helical spin structure which can be transformed by a magnetic field into a conical and even a parallel configuration. Close to the ordering temperature a skyrmionic A-phase exists. SQUID magnetization and Mössbauer-spectroscopic measurements on $\text{Mn}_{1-x}\text{Co}_x\text{Si}$ and $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$ have been performed to determine the magnetic phase diagrams. For a critical substitution of Co ($x_{\text{Co}} \approx 0.08$) and Fe ($x_{\text{Fe}} \approx 0.15$) the ferromagnetic order in MnSi is suppressed. Small angle neutron scattering gives an indication for a spin-glass state above the critical concentrations. The intermixing compound $\text{Mn}_{1-x}\text{Fe}_x\text{Ge}$ has been magnetically characterized for the first time. A preliminary determination of the magnetic phase diagram for different Fe-concentrations has been created. The monogermanides show a remarkably huge increase of the helix period from 3 nm for MnGe up to 70 nm for FeGe compared to 18 nm for MnSi, and the critical fields H_{C1} and H_{C2} increase from MnGe towards FeGe by the factor of 10.

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Isothermal structural transition in $\text{Bi}_{1-x}\text{La}_x\text{FeO}_3$ V.Sikolenko^{1,2}, M.Tovar², D.Többers², V.Efimov³, M.Bushinsky⁴, D.Karpinsky⁴ and I.Troyanchuk⁴

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BiFeO_3 is a very rare example of a single-phase material in which ferroelectricity, antiferromagnetism and ferroelasticity coexist in a broad temperature range. We have investigated the $\text{Bi}_{1-x}\text{La}_x\text{FeO}_3$ system [1,2] in a broad range of lanthanum concentration in a broad temperature range using upgraded high resolution neutron diffractometer E9 in Helmholtz Centre Berlin.

At room temperature an initially pure polar rhombohedral phase gradually transforms into a pure antipolar orthorhombic one. The polar phase can be recovered by annealing at $T > 300^\circ\text{C}$. An inverse isothermal antipolar-polar transition takes place at $T > 300^\circ\text{C}$, where the polar phase becomes more stable. The antipolar phase is characterized by a weak ferromagnetic state, whereas the polar state has been obtained in a mixed antiferromagnet-weak ferromagnet state.

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P68

High-resolution neutron spectroscopy of excitation lifetimes in solids

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The TRIPLe axis resonance SPin echo spectrometer (TRISP) at the FRM II neutron source in Garching near München, Germany has been used to study the momentum and temperature dependent lifetimes of acoustic phonons in elemental superconductors lead and niobium [1], showing the observed Kohn anomaly from both superconductors has exactly the same energy as the superconducting gap 2Δ at $T = 0$. This phenomenon was not anticipated by the standard theoretical framework for conventional superconductors. In addition, a detailed study on magnon lifetimes in prototypical antiferromagnet MnF_2 [2] has revealed that scattering from longitudinal spin fluctuations limits the magnon lifetimes over a wide range of temperatures. In this poster some of our more recent results on both magnetic excitations and phonons will be presented, and we will also describe the new sample environment capabilities now available for users at TRISP.

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P69

Diffusivity determination in bulk materials on nanometric length scales using neutron reflectometry

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A method that allows to measure ultra-low diffusivities in solids down to 10^{-25} m²/s is neutron reflectometry. Up to now this method was successfully used to study self-diffusion in isotope multilayer films [1,2]. Here, a new approach is presented in order to determine self-diffusivities in bulk materials on small length scales of 1 - 10 nm. The new method [3] is demonstrated for lithium self-diffusion in LiNbO₃ single crystals at low temperatures.

Lithium niobate (LiNbO₃) is a technologically important oxide with an extraordinary combination of ferroelectric, piezoelectric, acoustic, optical, and ion conducting properties. For many applications self-diffusion of the constituents is of high importance. Especially, the formation, stability and dissociation of defect clusters are closely related to diffusion properties close to room temperature.

For analysis with neutron reflectometry ⁶LiNbO₃ (amorphous film) / ^{nat}LiNbO₃ (single crystal) structures were used. Lithium diffusivities are derived from neutron reflectivity patterns in the temperature range between 125 and 250 °C. The results are in good agreement with those obtained by second ion mass spectrometry on the same type of samples but on larger length scales up to 90 nm, as given in literature [3,4]. In addition, neutron reflectivity simulations were performed in order to investigate the influence of diffusion length and scattering length density on the quality of the results. The limitation of the method is discussed.

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P70

Lithium transport through nano-sized silicon layers

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Lithium migration and intercalation are the basic processes for lithium based energy storage devices (accumulators, batteries). Miniaturisation is a demand for fabrication of portable electronics and electric vehicles. Properties of nanostructured building units can lead to novel technological perspectives [1-3].

We present a new approach to measure lithium permeability, solubility and diffusivity through nanometer thick films (1 to 20 nm) of relevant electrochemical materials. Measurements will be presented for lithium migration through nano-sized silicon layers (a potential electrode material) capped by nano-sized LiNbO₃ layers (a potential electrolyte material). For that purpose we fabricated superlattices with a repetition of five [⁶LiNbO₃ / Si / ^{nat}LiNbO₃ / Si] multilayer-units by ion beam coating. Each LiNbO₃ layer is separated by nano-sized silicon layers. The thickness of the LiNbO₃ layers was 10 or 15 nm. The thickness of the Si spacer layers was 15 nm. Sputtered LiNbO₃ is here used as Li tracer source.

Grazing incidence x-ray diffraction revealed that the LiNbO₃ and Si layers are amorphous. Auger electron spectroscopy and Raman-scattering evidenced the existence of elemental silicon. X-ray reflectometry, neutron reflectometry (NR) [4], cross-sectional scanning Auger electron microscopy and second ion mass spectrometry (SIMS) proved the LiNbO₃/Si material contrast. SIMS evidenced also the presence of the ⁶Li or ⁷Li isotope contrast in the LiNbO₃ layers. NR measured additional Bragg peaks appearing exclusively from the ⁶LiNbO₃ and ^{nat}LiNbO₃ isotope modulation of the superlattice. Li transport kinetics is determined non-destructively by NR.

Diffusion experiments were performed by heating the superlattices to 225 °C. During annealing the Bragg peaks resulting from ⁶Li / ^{nat}Li isotope modulation decrease, while that from the LiNbO₃/Si modulation remain approximately constant. This demonstrates that the Bragg peak decrease is a measure for the ⁶Li and ⁷Li intermixing through the Si layer by ionic diffusion. We anticipate that these preliminary results open the possibility to study the rate determining step (diffusion controlled or interface reaction controlled) of the Li transport process and the lithium permeability, solubility and diffusivity in various nano-sized membrane materials (metal, semiconductor or isolator) as a function of (i) chemical composition, (ii) film structure (amorphous or nanocrystalline), (iii) confinement (thickness of nano-layers) and (iv) space-charge effects [1-3].

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Real-time investigation of the structural evolution of electrode materials in a commercial lithium ion battery by neutron powder diffraction

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In-situ neutron powder diffraction was employed to investigate the structural evolution of the electrode materials in a commercial lithium ion battery used in electric buses in Taiwan. For the LiFePO_4 cathode in battery, a delayed phase transition between triphylite and heterosite was observed, but this phase delayed was not found in the $\text{LiFePO}_4\cdot\text{VO}_x$ cathode (see Fig. 1), suggesting that the delayed structural transformation could be eliminated by adding vanadium oxide into the pristine LiFePO_4 , which might enhance the capacity and prolong the cycling life. In the meanwhile, the structural change of the anode (Li_yC_6 for $0 < y < 1$) follows the Li/graphite voltage curves, and this process is readily reversible. LiC_6 is observed at the point where y increases to around 0.81.

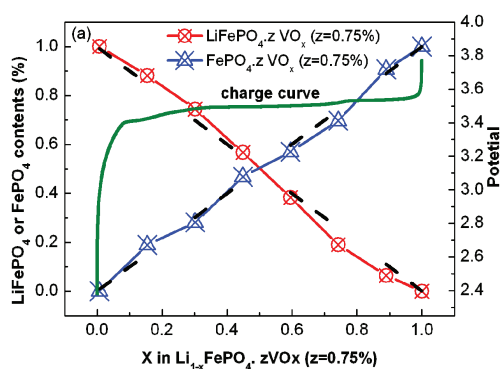


Fig. 1: The composition ratio of $\text{LiFePO}_4/\text{FePO}_4$ at different charging states of a $\text{LiFePO}_4\cdot\text{VO}_x$ Li battery.

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Recent experiments at the TOF reflectometer REFSANS

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The TOF horizontal reflectometer REFSANS was initially designed by the Helmholtz Research Center Geesthacht (now HZG, until 2011 GKSS) to study soft matter surfaces and interfaces. However it quickly appeared that this instrument can be used by a much wider scientific community. We will here present some recent experiments highlighting the potential offered by the combination of the TOF operation, a versatile collimation and an easily reconfigurable sample position. Examples will cover specular and off-specular reflectometry and GISANS (in-plane resolved off-specular) measurements on biological samples, polymer thin films, hybrid polymer/inorganic materials, and metallic multi layers.

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Robust Monte Carlo Fitting of Small-Angle Neutron Scattering Curves for Determining Cluster Size Distributions

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Reactor pressure vessel (RPV) steel, when exposed to fast neutron irradiation, leads to the formation of nano-sized clusters [1]. These clusters can cause an overall degradation in mechanical properties, which is a safety issue. Small-angle neutron scattering (SANS) is a commonly used technique to determine the irradiation-induced cluster volume fraction and cluster size distribution in the material.

However, in the case of modern RPV steels, standard data treatment [2] for back-transforming the SANS scattering curves to real space can lead to unstable results. These are highly dependent on renormalisation parameters to be chosen by the user.

Here, a Monte Carlo fitting (MCF) algorithm based on [3] is presented. No renormalisation parameter is needed. The algorithm is optimized to get a robust determination of small cluster volume fractions ($\approx 0.01\%$) and cluster radii (≈ 0.7 nm), which are typical for modern RPV steels. The significance of the resulting data can be evaluated by an automatic error analysis. Using simulated scattering curves, the MCF is able to deliver a good reconstruction of the cluster size distribution and volume fraction in the vicinity of the SANS detection limit. Furthermore, the algorithm is tested with experimental scattering curves of neutron-irradiated RPV steels. The MCF transformation yields in physical meaningful, non-divergent results. Comparisons between analyses performed by the standard methods [2] and the MCF algorithm are drawn. The stability of the results and the limits of information to be extracted from the experimental data are discussed.

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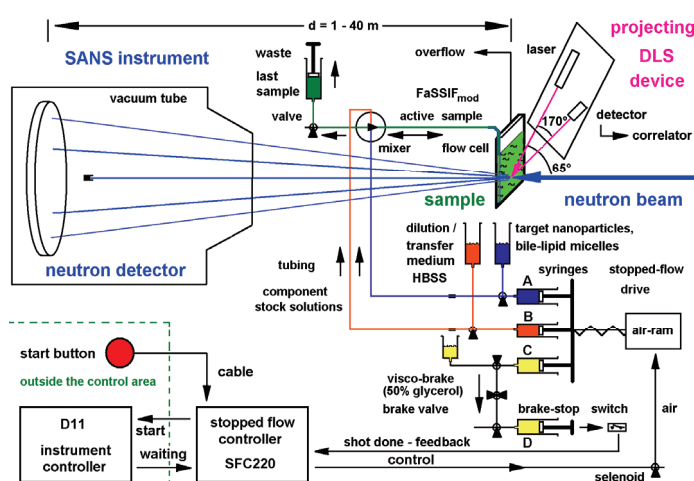
Combined SANS and DLS time-resolved study of a Bile-lipid model system for drug administration

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Setup for time resolved double beam SANS+DLS investigation at the improved instrument D11 at the ILL [1]

Oral administration is the most frequent way of pharmaceutical drug administration. Many new drugs are lipophilic or badly soluble, which results in a dependence of the uptake by interaction with dynamic nanoparticle-bile systems in the gastro-intestinal system. The formation and drug delivery of those nanoparticle systems can be studied with model systems.

The FeSSIF, FaSSIF models [2] simulate the human bile fluid and the gut content after bile influx. We use these systems for the simulation of drug uptake in the body, and development of formulations, which shall enable the administration of new drugs with bad solubility or gut permeability, i.e. drugs of the BCS classes 2, 3 and 4. The key step of those processes is the formation of dynamic nanoparticles in the gut with bile, which are mixed lipid-bile-drug micelles and liposomes. These trigger the uptake, e.g. as a lipid-drug co-transport. Formation, destruction and composition of those nanoparticles are investigated by SANS with D-contrast and dynamic light scattering. The figure shows our novel setup for simultaneous SANS+DLS investigation at ILL-D11. The results [1] indicated the formation of liposomes during 1 minute after bile influx in the gut, and of a temporal species of mixed micelles at 10 seconds. The application with drugs and addition of uptake adjuvant formulations shall solve the bioavailability restrictions of BCS class 2,3,4 drugs, which are important medical problems now.

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P75

Development of Novel Neutron Detectors with Thin Conversion Layers in Inclined Geometry

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The Helmholtz-Zentrum Geesthacht (HZG) operates neutron beamlines at the research reactor FRM II in Germany and is engaged in designing new ones at high flux reactors and the forthcoming European Spallation Source ESS. For those instruments thermal and cold detectors covering a large part of the spatial angle are needed. Due to the shortage of ³He HZG has started a development of neutron detectors with thin boron conversion layers to be used for high and low resolution diffraction, reflectometry and SANS as well as for inelastic instruments.

The new detectors are required to meet or even to surpass the high performance of current ³He-detectors, this includes especially high neutron and low Gamma sensitivity as well as high local and global count rates. A basic design concept of the new detectors is that neutrons hit conversion layers at small angles (inclined geometry). This distinguishes them from other ones. The inclined geometry of incident neutrons toward converter plates gives rise to an excellent detection probability and high angular as well as high timing resolution. Two different kinds of these novel detectors are designed. Those for elastic diffractometers have high spatial resolution (less or about 1 mm × about 2 mm) and shall allow for covering medium sized areas (up to 1 m²), whereas those for inelastic instruments have low resolution (about 10 mm to 20 mm) are designed to cover large areas (some 10 m²).

The development comprises i) the production, characterization and optimization of thin layers with high Boron content, ii) testing the quantum efficiency of these conversion layers in test detectors, and iii) the development of prototype detectors in which sets of thin 2D-lamellar detector elements are operated simultaneously. The currently achieved performance (e.g. quantum efficiency, spatial resolution and Gamma sensitivity) of the test detector with ^{nat}B₄C and ¹⁰B₄C converter samples as well as first tests of operation of adjacent detector elements in the prototype detector are presented - the development of the conversion layers is subject of a further contribution. The development is performed as an in-kind contribution to the ESS instrumentation, and is part of the German support to the ESS Pre-Construction Phase and Design Update.

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Magnetron sputter deposition of B₄C conversion layers for neutron detection

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The Helmholtz-Zentrum Geesthacht (HZG) possesses a strong expertise in x-ray mirror development and is equipped with a unique sputtering facility, which is able to manufacture precise and up to 1.5 m long coatings. This tool is employed to develop B₄C conversion layers, which can be an alternative to the ³He-based detectors. The challenge is to deposit adhesive, stable, continuous, ¹⁰B-enriched and µm-thick B₄C layers on aluminium plates, which will be installed in a novel detector system based on an inclined geometry.

B₄C layers were first coated onto small silicon substrates to study the layer properties. A very thin bonding layer of titanium improved the film adhesion. After optimization of the sputtering conditions, a B₄C layer thickness of about 2 µm was achieved. The film thickness and elemental composition were investigated by means of stylus profilometry and surface analysis. The thickness deviation is below 4% over the whole deposition area. The ratio of B/C amounts to 3.6, which is nearly similar to the target content. The film-substrate combination exhibits compressive stress of about 3 GPa that is determined by curvature measurement. Annealing experiments indicate that it is possible to reduce the film stress after the deposition. Relaxation processes lead to a decrease in film curvature.

Recently, B₄C conversion layers were deposited on aluminium plates. A pre-treatment of the surface was acquired to manufacture the coatings directly without any bonding layer. Using optimized deposition conditions, the maximum thickness is enhanced to 3 µm. The elemental and isotopic composition of B₄C on Al was measured and depth profiled. First neutron experiments are performed with up to 3 µm thick ¹⁰B₄C coatings. The first and promising results on quantum efficiency are presented by the contribution of R. Kampmann. In the near future, the good progress will be exploited to fabricate ¹⁰B-enriched B₄C conversion layers. The development is performed as an in-kind contribution to the ESS instrumentation, and is part of the German support to the ESS Pre-Construction Phase and Design Update.

P77

The new measurement of the electric dipole moment of the neutron at the FRM II

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Since the 1950's people search for electric dipole moments (EDMs) of fundamental particles. A non-zero value of an EDM would correspond to a manifestation of a broken symmetry at high energies and thus show that there is physics beyond the Standard Model. Although experimental searches for EDMs are among the most precise measurements in physics, no EDM has been observed so far. In this talk a next generation approach based at the FRM-II neutron source will be discussed. We project to achieve a systematic and statistical limit of $5 \cdot 10^{-28}$ ecm at 3σ confidence level on a competitive time-scale. To achieve this goal, Ramsey's method of separated oscillatory fields is applied to trapped ultra-cold neutrons in vacuum. For the investigation of systematic effects a sophisticated system of various means to control ambient disturbances is currently being set up. An overview of the strategy, main systems for magnetic field control and magnetometry, as well as the current status of the ongoing implementation on site will be shown.

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WITHDRAWN

P79

Large Sample Neutron Activation Analysis using isotopic: Neutron Source: Monte Carlo simulation

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Prompt gamma neutron activation analysis (PGNAA) is mostly done with (cold) neutron beams, taking advantage of the relatively high neutron intensity [1]. PGNAA with radio-isotopic neutron sources (^{252}Cf , $^{241}\text{Am-Be}$ or $^{239}\text{Pu-Be}$) is used intensively for on line and in situ analysis in various fields (industry, oil exploration, coal, concrete analysis etc.) [2-4]. The relatively low neutron fluence rate is often compensated by exposing large amounts of material to the neutrons. Most applications deal with solid materials but in principle the PGNAA can also be applied to liquids. A research project was initiated to assess the feasibility of isotopic source based PGNAA as a field method for screening of water for specific contaminants. In previous work [5] we reported already on the use of calculations for estimating the fluence rate and energy distribution of the neutrons in a voluminous water sample, emitted by an $^{241}\text{AmBe}$ source. In the present work, these MCNP calculations [6] have been extended to the estimation of the Ge-detector efficiency. These calculations have been experimentally verified for the determination of cadmium (as an example) in a water sample. Given the overall objective, the development of a fast screening technique, a pragmatic approach was developed for the estimation of the concentration of elements present in a water sample based simply on the simulation of the thermal fluence rate and the detector efficiency. To this end, it has been explored if the water's hydrogen could be used as an internal calibrator. For validation, the concentration of cadmium in water was found similar to known amount dissolved in water and irradiated by the $^{241}\text{Am-Be}$ source. The simulation with MCNP code will be used to estimate the concentrations of pollutants without resorting to costly experimental trials in travel time on site and equipment.

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P79A

Dynamic consequences of missing chain ends in cyclic polyethylene glycol

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The dynamic behaviour of cyclic polymers arouses great interest due to the absence of chain ends [1]. Since the relaxation mechanisms of linear polymer chains are strongly influenced by their chain ends cyclic polymers are expected to show significantly different dynamics. Furthermore the structure of cyclic polymers differs from linear polymer chains. In a melt cyclic polymers assume more compact conformations than their simple linear analogues of Gaussian chains do. This has a serious impact on the general properties of ring polymers, independent of the detailed monomer chemistry.

A synthetic approach established in-house allows to increase the purity of cyclic polyethylene glycols by adding a second purification step sensitive to linear impurities compared with the conventional synthesis [2]. By this reasonable amounts to perform neutron scattering experiments in the melt could be obtained. Therefore the comparison of theoretical approaches and simulations on cyclic polymers with experiments is possible for the first time on a microscopic scale. With this contribution we will give an overview of the investigation of two different molecular weights. The lower molecular weight is below the entanglement molecular weight M_e of the corresponding linear chain [3], the second polymer investigated is above M_e where the onset of entanglements comes into play for the linear chain. The dynamic behaviour found is in good agreement with recently published MD simulations on cyclic polyethylene of comparable chain length in respect of the linear M_e [4]. Whereas the present study on pure architectures already deals with the fundamentals of what entanglements are and the effect of chain ends on the dynamics in view of a unified description, also the investigation of blends of ring polymers and linear chains has become of utmost importance. These are neither understood nor theoretically predicted and new developments will be required in the future.

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P80

Time-Resolved SANS Experiments for the Understanding of Structural Transitions in Self-Assembled Systems

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The static structural properties of self-assembled systems are well established by now. In contrast, their dynamic properties and the structural transitions that may occur upon changing external parameters such as temperature, pressure, or sample composition have been studied to a much lesser extent. However, such transitions are very important for the understanding of self-assembled systems, for instance with respect to their release and solubilisation properties as well as for controlling the structural formation in non-equilibrium systems.

As one example we studied in some detail the process of vesicle formation as it occurs upon mixing anionic surfactants with cationic or zwitterionic surfactants. The structural progression can be followed by coupling the stopped-flow mixing with time resolved SANS [1] or SAXS [2]. From these experiments we can conclude that the formation process proceeds via intermediate disk-like micelles that close to form very monodisperse unilamellar vesicles, where this monodispersity is controlled by the formation process, i.e., it takes place under kinetic structural control. This process can be simulated by means of appropriate diffusion-based models and thereby the whole formation process can be put on a sound theoretical understanding. Based on the knowledge of the formation process we are then able to modify this process by admixture of appropriately chosen amphiphilic copolymers and thereby control size and stability of the formed vesicles [3].

As a second example we investigated the solubilisation dynamics in micro- and nanoemulsions by means of time-resolved SANS experiments. They show that the solubilisation dynamics depends in a subtle way on the surfactant monolayer employed. It is controlled by the molecular architecture of the surfactants present there, as that determines the bending elasticity of this amphiphilic monolayer.

In summary, it can be stated that understanding the dynamic aspects of self-assembled systems is the key for a better understanding of their properties and their applications, as well as for shaping more complex self-assembled structures.

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The Geometrical Shape of Micelles Formed By Cationic Dimeric Surfactants Determined with Small-Angle Neutron Scattering

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The influence of spacer group on the geometrical shape of micelles formed by quaternary-bisdimeric (Gemini) surfactants $C_{12}H_{25}N(CH_3)_2(CH_2)_sN(CH_3)_2C_{12}H_{25}$ (12-*s*-12) have been investigated with small-angle neutron scattering (SANS). Dimeric surfactants with a short spacer unit (12-3-12 and 12-4-12) are observed to form oblong general ellipsoidal micelles with half axes $a < b < c$, whereas SANS data demonstrate that rather small spheroidal micelles, rather than strictly spherical micelles, are formed by dimeric 12-*s*-12 surfactants with $6 \leq s \leq 12$. Moreover, by means of comparing our present SANS results with previously determined growth rates, using time-resolved fluorescence quenching (TRFQ), we are able to conclude that micelles formed by 12-6-12, 12-8-12, 12-10-12 and 12-12-12 are shaped as oblate rather than prolate spheroids. Hence, our investigations suggest a novel structural behavior of Gemini surfactant micelles, according to which the micelles transform from oblong ellipsoids to oblate spheroids as the length of the spacer group is increased. The micelle aggregation number is observed to monotonously decrease with an increasing length of the surfactant spacer group, mainly as a result of a decreasing half axis related to thickness (*a*) of the micelles, whereas the half axis related to width (*b*) is rather constant with respect to *s*. We argue that geometrically heterogeneous elongated micelles are formed by dimeric surfactants with a short spacer group, mainly as a result of the surface charges becoming less uniformly distributed over the micelle interface. As the length of the spacer group increases, the distance between intra-molecular charges become approximately equal to the average distance between charges on the micelle interface and, as a result, rather small oblate spheroidal micelles with a more uniform distribution of surface charges is formed by dimeric 12-*s*-12 surfactants with $6 \leq s \leq 12$.

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A SANS study of the solution structure of patchy worm-like micelles

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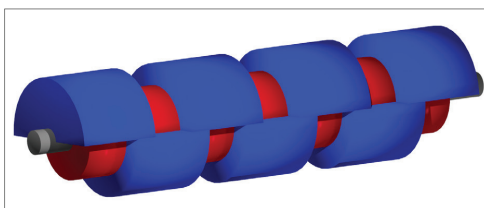
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The self-organization of triblock terpolymers provides a smart way to obtain hierarchically self-organised nanostructures including the formation of fascinating cylindrical core-shell systems with a phase separated corona. The crystallization induced self-assembly of polystyrene-*b*-polyethylene-*b*-poly(methyl methacrylate) triblock terpolymers in solution leads to wormlike core-shell micelles exhibiting a patchy corona of polystyrene and poly(methyl methacrylate) which could be observed via transmission electron microscopy using staining techniques [1]. However, the morphology in solution remains still unclear. Here we present a SANS study with contrast variation performed on a triblock terpolymer with deuterated styrene-blocks. This method enables us to focus on only one compartment of the corona. Furthermore, it provides the possibility to distinguish in-situ between a Janus-type (two faced) and a patchy (multiple compartments) configuration of the corona. The results validate the existence of the patchy structure also in solution.



Model of the patchy worm-like micelles

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Time-resolved SANS studies on the guest exchange process in crystalline complexes of syndiotactic-polystyrene

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Syndiotactic polystyrene (sPS) is a relatively new commodity polymer, which exhibits a variety of solid states. One of the important properties of sPS is the formation of complex crystalline states, where a wide range of chemical compounds including functional molecules can be stored into the cavities between polymer sheets consisting of TTGG helices [1-4]. The guest in the cavities is easily substituted with another compound by exposing the complex sPS film to its vapour or liquid, keeping the framework of the host sPS crystallites. Now sPS crystalline complexes are regarded as of high potential for polymer based composite materials. Exploiting the difference in molecular scattering length between two isotopologues, fully protonated (H) and deuterated (D) forms, employed as old and new guests, we started to investigate the characteristics and mechanism of the guest exchange through time-resolved high intensity SANS at FRM II neutron source in Garching-München. The in-situ crystallization and guest exchange process could be followed in this case by measuring the reflections due lamellar structures with uniaxially oriented samples. Recent SANS experiments revealed that the exchange between protonated and deuterated isotopologues proceed smoothly, keeping the higher order structure of the sPS crystalline region. In particular, the exchange process was completed within several minutes for many small chemical species, as chloroform, benzene, toluene or tetrahydrofuran. The replacement from protonated guests to deuterated ones, and vice versa, caused significant changes in SANS profile, from which the time dependence of the one-dimensional correlation function $\rho(x)$ could be evaluated. The $\rho(x)$ data delivered the information about the rate of exchange as well as how the distribution of old and new guests in the lamellae varies during the exchange process. The analysis of $\rho(x)$ suggested that the exchange proceeds from the lamellar surface region to the interior.

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P84

Mesoscopic magnetic structure and competing anisotropies in laterally patterned Fe/Cr-layer systems

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Patterned magnetic structures are the basic elements of spintronic devices. The ongoing miniaturization makes the influence of neighboring structures more and more important. Fe/Cr multilayers have been grown epitaxially on GaAs (100) single crystals by Molecular Beam Epitaxy. The Cr interlayers induce an antiferromagnetic coupling between adjacent Fe layers. Thus, the magnetic dipole moment is reduced and a magnetic superstructure is created, which is, due to the contrast of Cr to Fe, easily observable by polarized neutron reflectometry. The lateral structuring was performed by UV-nanoimprint lithography and Reactive Ion Etching. The structural characterization was carried out by Scanning Electron Microscopy, Atomic Force Microscopy and X-ray scattering under grazing incidence. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. Polarized neutron reflectometry and off-specular scattering was used to determine the magnetic domain formation within the individual layers. Furthermore, simulations of the neutron data were generated and compared with the measurement in order to improve the simulation model. The work presented gives insight into the interplay of shape and crystal anisotropy within the individual layers and patterns.

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Nano- and microstructure of thermoelectric PbTe alloys studied by small angle neutron scattering

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Thermoelectric devices, which can convert waste heat into electricity, may play a major role in achieving global sustainability. The quality of thermoelectric materials is usually evaluated in terms of the dimensionless figure of merit $ZT = \alpha^2 \sigma T / \kappa$, where α is the Seebeck coefficient, σ the electrical and κ the thermal conductivity respectively. Therefore, the fundamental challenge in developing good thermoelectric materials is related to the optimization of interdependent and partly conflicting material properties, namely low thermal conductivity in combination with good electrical conductivity. From the material science perspective, special attention is drawn on materials containing nanometer sized precipitates and materials exhibiting grains of similar size [1]. A crucial point is that internal surfaces made up by nano-precipitates or by grain boundaries are thought to act as effective phonon scattering centers. Among other means, the figure of merit of such materials can thus be raised by tuning the internal surface area.

Nowadays, great attention is drawn to systems based on the gold standard of conventional bulk thermoelectric materials for medium, $\sim 400^\circ\text{C}$, temperature applications, namely PbTe. Compounds of the systems PbTe-Sb₂Te₃ and PbTe-Ag₂Te₃ usually outperform their mother compound and allow for rich and complex nanostructures [2, 3]. Due to their tremendous complexity, samples of these compounds were investigated by small angle neutron scattering, in order to access their nanostructure in an integral way. Thus, a correlation between global parameters of the nanostructure such as the internal surface area or the size distribution of particles and thermoelectric parameters can be attempted in a quantitative way.

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P86

Induced Magnetisation in Pd/Fe-Multilayers

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Proximity effects in magnetic multilayers give rise to new physical properties which are interesting for new spintronic devices. Because of a high Stoner parameter of 0.78, Pd almost fulfils the Stoner criterion for ferromagnetism and makes this material especially interesting. Due to hybridization with a magnetic material like Fe it is possible to induce a magnetic moment into the Pd layer [1,2].

Therefore we prepared epitaxial Pd/Fe multilayers with a varying layer thickness of Fe with molecular beam epitaxy. These films were investigated with SQUID magnetometry, X-ray reflectometry and polarized neutron reflectometry.

X-ray reflectometry measurements show a low surface roughness with sharp interfaces between Pd and Fe and therefore nearly no interdiffusion. Assuming that the whole magnetic moment is due the magnetic moment of Fe, the SQUID magnetometry measurements show an increase of the Fe magnetic moment with decreasing Fe layer thickness. This can be attributed to a small magnetic polarization of Pd whose relative weight increases with thinner Fe layers. The polarized neutron reflectometry measurements could not distinguish between models with and without magnetic polarization of Pd but additional neutron measurements are planned with a better signal to noise ratio.

We will present the results of the SQUID, X-ray and neutron measurements.

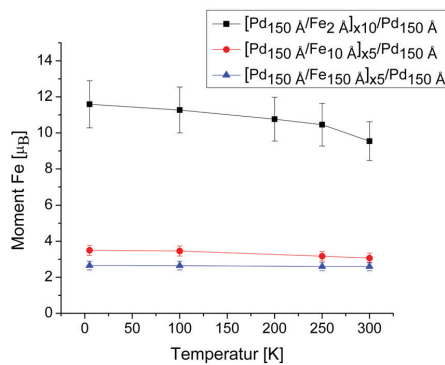


Figure 1: SQUID measurements. The magnetic moment from measured hysteresis is assigned only to the magnetic moment of Fe.

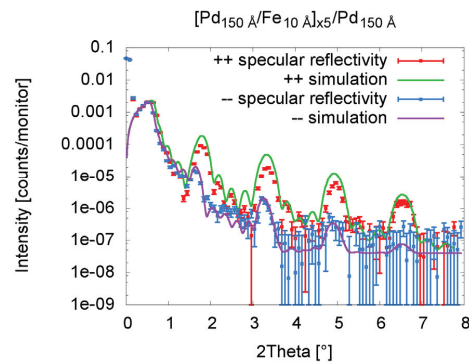


Figure 2: Polarized neutron measurements with magnetically saturated samples and simulations thereof.

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Spindynamics in $\text{CaBaCo}_2\text{Fe}_2\text{O}_7$ under strong geometrical frustration

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Recent studies of spin correlations in new materials belonging to the swedenborgite compound family ($P6_3mc$) [1] exhibit signs of unusual strong geometric frustration: at low temperatures, indications for quasi 2D spin correlations, spin glass or spin liquid states, and also rather complex, partly ordered ground states have been observed.[2–5] Several groups have investigated this compound family with different stoichiometry, however, up to date the main focus has been on solving structural and ground state configurations (f.e. [6]).

Since the material characteristics are dominated by the strong magnetic frustration, excitations are very sensitive to small changes in ordering and exchange interactions. We will present neutron inelastic scattering on a single crystal of the compound $\text{CaBaCo}_2\text{Fe}_2\text{O}_7$, that have been obtained from triple axis (PANDA) and thermal time-of-flight scattering (ARCS). The experimental results will be discussed in comparison with theoretical calculations of the phase diagram and the spin dynamics based on nearest neighbor Heisenberg models.

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Neutron diffraction on highly stoichiometric YFe₂O_{4-δ} single crystals

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LuFe₂O₄ was long time attracting attention as proposed multiferroic compound, but there is much less known about other isostructural rare-earth ferrites. We have grown single-crystals of YFe₂O_{4-δ} in a CO/CO₂ atmosphere to tune δ. Optimized crystals exhibit, for the first time, a magnetic behavior identical to highly stoichiometric powder samples [1], i.e. two hysteretic phase transitions at 228 K and 180K upon cooling, compare Fig. 1.

We observed four different 3D-charge-ordered phases in single crystal x-ray diffraction down to liquid nitrogen temperature, totally different to LuFe₂O₄.

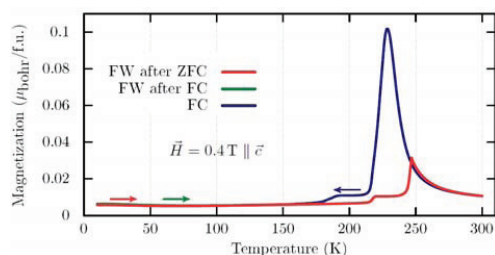


Fig. 1 Magnetisation of YFe₂O_{4-δ}

Neutron diffraction, done at the JCNS DNS instrument on a 50mg YFe₂O_{4-δ} crystal, shows 3D-magnetic ordering below the Néel-Temperature (see Fig. 2). This is in contrast to non stoichiometric samples where magnetic ordering stays two dimensional down to 10 K [2]. Above the Néel-Temperature diffuse magnetic scattering along (1/3,1/3, ℓ) is observed as in LuFe₂O₄ [3], indicating broken long range interlayer correlation.

With neutron polarization analysis we probed the direction of the magnetic moment in stoichiometric YFe₂O_{4-δ}. While in the 3D-ordered phase the system is purley Ising with the hexagonal c-axis as the easy axis, in the 2D-ordered phase in plane contributions are present. Two different magnetic 3D-ordered phases are observed, which consist of peaky lines slightly incommensurable shifted from (1/3,1/3, ℓ). The incommensurability is strongly temperature dependent.

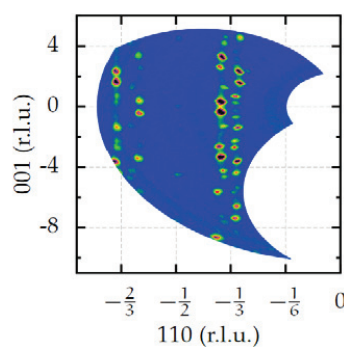


Fig. 2 Spin-flip P || [1 -1 0]

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P89

Lattice Dynamics of Pure and Impure Nanocrystalline Si for Thermoelectric Applications

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Thermoelectric materials can be used for waste heat recovery by converting a heat flow into electricity and vice-versa. The figure of merit ZT , which governs the conversion efficiency, is dependent on the Seebeck coefficient, electrical conductivity and inversely proportional to the thermal conductivity of the material. Different approaches are used in order to increase ZT , namely enhancement of electrical properties and reduction of thermal conduction, which can be achieved through nanostructuration. Silicon is a well studied and unexpensive material that could be used in thermoelectric devices for waste heat recovery at high temperatures, however its bulk thermal conductivity is too large and limits its performance. Therefore the production of nanocrystalline Si and the influence of nanostructuration upon the lattice dynamics is of great interest. In this work, different batches of phosphorous-doped Si nanoparticles were synthesized by a plasma assisted gas phase process, using a microwave reactor. By changing the microwave power, the chamber pressure and/or the concentration of the precursor and plasma gases it was possible to produce different sizes of nanoparticles. Some of the batches were exposed to air while others were kept in an inert atmosphere. The compaction of the Si nanoparticles into a pellet was done with spark-plasma sintering. Structural analysis of the samples was done by TEM, XRD and PDF. The lattice dynamics of nanocrystalline Si pellets was extensively studied through measurements of the elastic constants, heat capacity, thermal conductivity and density of phonon states with neutron inelastic scattering. Samples for which the nanopowder was exposed to air before sintering reveal a boson peak in the heat capacity and in the reduced density of phonon states, a peak that corresponds to vibrational states above the Debye level usually observed in glasses. It is indicative of the presence of amorphous SiO_2 , and was not observed on the samples kept under inert atmosphere. The nanocrystalline silicon samples with amorphous SiO_2 present a significant reduction of the thermal conductivity, up to 90% with respect to the bulk material, a decrease that yields a ZT three times larger than the bulk material.

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Wide angle ^3He neutron spin filters

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Polarization analysis is very useful for soft matter research. Removal of incoherent background can reduce the number of parameters need to fit data, especially in the high-Q regime. We have been working on an ultra compact ^3He polarizer to be used as a polarization analyzer for this purpose. The ^3He will be polarized in-situ within a very compact magnetic cavity, 18 cm long, that can be simply placed between the sample and the detector tank without lowering the maximum achievable Q range of the SANS machines we currently use at the JCNS. The angular coverage is a pyramid of 38° from the sample position. The optical pumping will be done with an ultra compact volume Bragg grating frequency narrowed diode laser array bar. The full system will be readily hand transportable and thus useful as an instrument add-on.

We present also a finite element calculation of the magnetic field (MagNet software) taken with the newly proposed PASTIS Coil, which uses a wide-angle banana shaped ^3He Neutron Spin Filter cell (NSF) to cover a large range of scattering angle. The goal of this insert is to enable XYZ polarization analysis to be installed on the future thermal time-of flight spectrometer TOPAS.

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11:00 - 11:15 h Welcome		
	10:30 - 11:00 h – COFFEE BREAK	
11:15 – 12:30 h Hydrogen Chemistry and Energy	11:00 – 12:30 h Soft Matter	11:00 – 12:30 h Information Technology and Magnetism II
12:30 - 14:00 h – LUNCH		
14:00 – 15:30 h Material Science	14:00 – 15:00 h Advanced Methods	14:00 - 15:30 h Instrumentation
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