Technische Universität München

Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

Technische Universität München

USER MEETING

30. October 2007

User Office
Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)
Technische Universität München
D-85747 Garching
Germany
Internet: http://user.frm2.tum.de
email: userinfo@frm2.tum.de
Phone: +49 89 289 14313

Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

First user meeting

30. October 2007, lecture hall LMU, Coulombwall 1, 85748 Garching

P R O G R A M

10:00	Registration
10:30	Welcome, Current and future instrumentation at the FRM II, W. Petry
11:00	The instrumentation of the JCNS at the FRM II, A. Ioffe
11:30	Around the weld in a few seconds with Stress Spec, R. Wimpory
12:00	Neutron diffraction studies on Li-ion battery materials, H. Ehrenberg
12:30	Development of Ni-Fe-al based alloys for fabrication of nanoporous membranes, F. Schmitz
13:00	Lunch
14:00	Spectroscopy and magnetism - A summary, T. Keller
14:30	Magnetic excitations in multiferroic $TbMnO_3$, D. Senff
15:00	Non-fermi liquid metal without quantum criticality, Chr. Pfleiderer
15:30	Coffe break
16:00	Inelastic spectroscopy for soft matter research, T. Unruh
16:30	Structural investigation of thin polymer films with TOF-GISANS at REFSANS, P. Müller-Buschbaum
17:00	Neutron diffraction - hot topic for more than 60 years, M. Meven
17:30	Simultaneous antiferromagnetic $Fe3^+$ and $Nd3^+$ ordering in $NdFe_3(^{11}BO_3)_4$ investigated by single crystal neutron diffraction at Heidi/FRMII and DMC, TASP&TriCS/SINQ, J. Schefer
18:00	The aSPECT spectrometer, R. Munoz Horta
18:30	Poster session , foyer Physics Department, James-Franck-Strasse 1 (incl. Buffet), open end (21:00)

1 Talks

1.1 Winfried Petry (FRM II): Welcome address, Current and future instrumentation at the FRM II

Since the start of the routine operation in May 2005 a large number of experiments could be performed at the FRM II. The still increasing number of instruments available cover a broad range of applications. An overview of the possibilities at the FRM II will be given by A. Ioffe, T. Keller, T. Unruh and M. Meven. With the inauguration of the Neutron guide hall east in 2007 we have opened the possibility for further instruments in the near future. In addition to the instruments special focus will be given to the infrastructure for experiments, namely sample environment and laboratories for users.

1.2 Alexander Ioffe (FZ Jülich):The instrumenation of the JCNS at FRM II

After the shutdown of the Jülich research reactor FRJ-2 in May 2006, a large part of its neutron scattering instrumentation have been moved to the reactor FRM II in Garching and the Jülich Centre for Neutron Science (JCNS@FRM II) has been established. An overview of the JCNS neutron scattering instrumentation will be given: they have undergone through major upgrades, which together with much higher flux available at FRM II have dramatically enhanced their performance.

1.3 Robert Wimpory (Hahn Meitner Institut): Around the Weld in a few seconds with Stress Spec

In recent years the main wishes 'buzz words' that are expressed the most with respect to neutron strain scanning are: accuracy, speed, user friendliness, efficiency, flexibility and better spatial resolution. Since Stress-Spec's first experiments in 2005 these wishes have been fulfilled and new developments are on the way to improve these still. The measurement and analysis of residual stresses, especially in weldments has gained significant importance. This talk involves the many measurements that have been made on weldments of many different geometries together with 'round-robin' exercises that have allowed Stress-spec to be compared with other instruments in a very favourable light.

1.4 Helmut Ehrenberg(IFW Dresden): Neutron diffraction studies on Li-ion battery materials

Neutron diffraction offers unique possibilities for the structural characterisation of electrode materials in Li-ion batteries, especially for the determination of Li- and oxygen positions and of the occupation factors on the corresponding sites. An investigation of the Li-extraction mechanism from $LiCoPO_4$ will be reported. In addition, the capabilities of the powder diffractometer SPODI for the determination of magnetic structures, even in the case of a multiphase sample, will be demonstrated for electrochemically delithiated $CoPO_4$.

1.5 Fabian Schmitz(TU Braunschweig, Institut für Werkstoffe): Development of Ni-Fe-Al based alloys for fabrication of nanoporous membranes

Nanoporous membranes showing very fine and regular porosity are desired for a great variety of functional applications such as filters in hospitals or as structures in miniature heat exchangers. In a new method the porous metal is produced from binary or multi-component alloys containing second phase precipitates. For the fabrication two phase alloys are subjected to a unidirectional external loading at elevated temperature. In the so called rafting process the cubic $\gamma\prime$-precipitates start to coarsen and finally create a network within the gamma-matrix. The initial precipitate arrangement and its morphology in the bulk alloy are important factors which guide their self assembly. In a following electrochemical leaching process one of the phases can be removed leaving the nanoporous membrane. So far, we have used commercially available single crystalline nickel-base superalloys for producing thin nanoporous membranes. Now research is in progress to produce the nanoporous membranes from polycrystalline alloys of simpler composition. The lattice misfit between the gamma-matrix and the $\gamma\prime$-precipitates is an important design parameter in the development of the new alloy. It controls the initial shape and distribution of the precipitates, the self assembly works best on systems having cubic precipitates which are well aligned. Neutron diffraction is the most suitable technique to determine the misfit in these alloys. The transmission geometry at SPODI enables us to get a full spectrum showing superlattice peaks as well as fundamental peaks even in textured specimen. Additionally a large volume of bulk material is measured, so that an overall misfit value is determined. The possibility to use different sample environments, especially a vacuum furnace and a tensile testing machine offer the possibility to monitor the changes of the misfit in all stages of the membrane fabrication.

1.6 Thomas Keller(MPI Stuttgart): Spectroscopy and Magnetism – a summary

K. Hradil, T. Keller,P. Link, R. Georgii, A. Rühm

We give an overview of recent experiments at the spectrometers PUMA, PANDA and TRISP, the reflectometer N-REX$^+$, and the multi purpose instrument MIRA. The examples are mainly limited to spin excitations. Recent upgrades of the instruments are presented.

1.7 Daniel Senff(II. Physikalisches Institut, Universität zu Köln): Magnetic Excitations in Multiferroic TbMnO3

The observation of a strong magnetoeleastic coupling in the last few years in a variety of compounds has lead to numerous work in the field of multiferroic oxides. Of particular interest is the magnetic excitation spectrum of such compounds, as it has been shown already 20 years ago [1], that the critical fluctuations of magnetoelectric systems are no longer of phononic character, as in ordinary ferroelectrics, but are composed of hybridized magnon-phonon excitations, frequently referred to as electromagnons. In a series of experiment on the two triple-axis spectrometers PANDA and PUMA we have analyzed the spin-wave spectrum of the multiferroic compound TbMnO3, which is one of the key elements in the class of multiferroic oxides. The emergence of the spontaneous electric polarization is closely correlated to the existence of a non-collinear, cycloidic magnetic structure. Our detailed investigation of the magnon excitations in TbMnO3 reveals the different character of the various spin-wave branches in the spiral structure, and the comparison with recent IR-spectroscopy results allows for the first time the experimental observation of the hybridized electromagnon excitations [2,3]. We will discuss the dispersion of these modes, as well as their field and temperature dependence.

[1] **G.A. Smolenskii and I.E. Chapuis, Sov. Phys. Usp. 25, 475 (1983).**
[2] **A. Pimenov et al., Nature Physics 2, 97 (2006).**
[3] **D. Senff et al., Phys. Rev. Lett. 98, 137206 (2007).**

1.8 Christian Pfleiderer(Technische Universität München, Physik Department E21): Non-Fermi Liquid Metal without Quantum Criticality

A key question in condensed matter physics concerns whether pure three-dimensional metals can always be described as Fermi liquids. Using neutron Larmor diffraction to overcome the traditional resolution limit of diffraction experiments, we studied the lattice constants of the cubic itinerant-electron magnet manganese silicide (MnSi) at low temperatures and high pressures [1]. We were able to resolve the nature of the phase diagram of MnSi [2,3] and to establish that a stable, extended non-Fermi liquid state emerges under applied pressure without quantum criticality. This suggests that new forms of quantum order may be expected

even far from quantum phase transitions.

[1] **C. Pfleiderer, P. Böni, T. Keller, U. K. Rößler, A. Rosch, Science 316, 1871 (2007)**
[2] **C. Pfleiderer, D. Reznik, L. Pintschovius, H. v. Löhneysen, M. Garst, A. Rosch, Nature 427, 227 (2004)**
[3] **C. Pfleiderer, S. R. Julian, G. G. Lonzarich, Nature 414, 427 (2001)**

1.9 Tobias Unruh (FRM II): Inealstic spectroscopy for soft matter research

A variety of user experiments on soft matter have already been performed at the neutron spectrometers of the FRM II. The investigated systems are as different as pharmaceutical nanodispersions and metalic melts or microemulsions and protein solutions. The dynamics of such systems can be studied in broad time and spatial ranges, namely from $\sim$0.01 ps to $\sim$350 ns and $\sim$0.02 Å^{-1} to $\sim$5 Å^{-1}, respectively, when combining the results from different spectrometers. Some selected experimental results and technical properties will be presented for spin-echo, backscattering and time–of–flight spectroscopy.

1.10 Peter Müller-Buschbaum(TU München, Physikdepartment E13): Structural investigation of thin polymer films with TOF-GISANS at REFSANS

Time-of flight (TOF) mode allows for a specular and off-specular scattering experiment, in which neutrons with a broad range of wavelengths are used simultaneously and registered as a function of their respective times of flight. Grazing incidence small angle neutron scattering (GISANS) overcomes the limitations of conventional small-angle scattering with respect to extremely small sample volumes in the thin film geometry. The combination of both, TOF-GISANS, enables the simultaneous performance of several GISANS measurements, which differ in wavelength. As a consequence, within one measurement a full set of GISANS pattern related to different scattering vectors and resolutions result, which allows the detection of nanostructures with a chemical sensitivity. Nanostructures parallel and perpendicular to the sample surface observable in thin polymer films are presented as an example of the possibilities of TOF-GISANS.

1.11 Martin Meven (FRM II): Neutron diffration – hot topic for more than 60 years

About 60 years ago, Brockhouse and Shull performed the first neutron scattering experiments worldwide (Nobel prize 1994). Since then, a lot of progress has taken place both in methological aspects (reactor techniques, instrumentation) as well as in the variety of applications for neutrons. The diffraction instruments as FRM II (HEIDI, RESI, SPODI, STRESS-SPEC) show the state of the art in this field of science. While HEIDI and RESI focus on single crystal diffraction with hot and thermal neutrons respectively, SPODI and STRESS-SPEC are designed for

powder samples and samples with powder like structures (grains) respectively. In the talk an overview will be given about the different designs of these instruments and some experiments results.

1.12 Jürg Schefer (ETH Zrich and Paul Scherrer Institut): Simultaneous antiferromagnetic Fe3$^+$ and Nd3$^+$ ordering in $NdFe_3(^{11}BO_3)_4$ investigated by single crystal neutron diffraction at Heidi/FRMII and DMC, TASP&TriCS/SINQ

J. Schefer(a), M Janoschek(a,c), V Pomjakushin(a), P Fischer(a), D Sheptyakov(a), L Keller(a), B Roessli(a), G Petrakovskii(b), L Bezmaternikh(b), V Temerov(b), D Velikanov(b), M. Meven(c)
(a) Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
(b) Institute of Physics, SB RAS, Krasnoyarsk 660036, Russia
(c) TUM, FRM-II, Munich

As promising materials for optoelectronics and with respect to interesting magnetic properties due to competing magnetic sublattices and magnetoelectric interactions, the family of borates $RM_3(BO_3)_4$ with R = rare earths or Y, La-Lu and M = Al, Ga, Cr, Fe, Sc is of current interest. $GdFe_3(BO_3)_4$ has been found [1,2] o exhibit a structural phase transition at 156 K, antiferromagnetic order of the magnetic Fe3+ moments at 36 K, followed by a spin reorientation phase transition at 9 K. Moreover there is evidence for an induced ferroelectric phase in this material in external magnetic fields which demonstrates a strong correlation between the magnetic order and the dielectric properties of $GdM_3(BO_3)_4$. Concerning technical applications such compounds, e.g. $YAl_3(BO_3)_4$, may be important materials for laser techniques and optical second harmonic generation [3]. By means of magnetic susceptibility and specific heat measurements, x-ray and unpolarized neutron diffraction investigations on powder and single-crystal samples, simultaneous long-range antiferromagnetic Fe and Nd ordering in $NdFe_3(^{11}BO_3)_4$ with R 3 2 chemical structure has been found at temperatures below $T_N = 30.5(5)$ K down to 1.6 K. At temperatures down to 20 K to the propagation vector is k_{hex} = [0,0,3/2] and becomes slightly incommensurate at lower temperatures. Symmetry analysis yields magnetic spiral configurations with the magnetic moments oriented parallel to hexagonal basal plane according to the irreducible representations τ3 in the commensurate case. This is in agreement with the easy directions of magnetization perpendicular to the c-axis as determined by magnetic susceptibility measurements. At 1.6 K the magnetic Fe moment amounts to 4.9 μB close to the free ion moment of Fe3+. The magnetic Nd3+ moment saturates presumably due to crystal-field effects at 2.7 μB [4]. There remains some doubt that the chemical structure is R3 instead of R 3 2, a problem most likely to be solved by neutron single crystal diffraction at TriCS/SINQ and HEIDI/FRM-2.

[1] **F. Yen, B. Lorenz et al., Phys. Rev. B 73 (2006) 054435**
[2] **S.A. Klimin, D. Fausti, A. Meetsma, L.N. Bezmaternyk, P.H.M. van Loosdrecht**

and T.T.M. Palstra, cond-mat/0502423 (2006)
[3] **M.H. Bartl et. al., Spectrochimica Acta A 57 (2001) 1981**
[4] **P. Fischer, V. Pomjakushin et al, J. Phys.: Condens. Matter 18 (2006) 7975.**

1.13 Raquel Munoz Horta(Institut für Physik - Universität Mainz): The aSPECT spectrometer

The purpose of the aSPECT spectrometer is a precision measurement of the proton recoil spectrum in free neutron decay. For kinematic reasons its shape depends on the angular correlation between the momenta of the antineutrino and the electron. Nowadays, a measurement of the antineutrino electron correlation coefficient a is of great interest in order to test the unitarity of the Cabibbo-Kobayashi-Maskawa-Matrix. First measurements with the aSPECT spectrometer have been performed in a beam time at the beam line MEPHISTO at the neutron research reactor FRM-II in Garching. A description of the spectrometer and first results of the data analysis will be presented.

2 Poster Experiments

2.1 Sohyun Park(LMU München): Study to ionic conductivity in the microporous lithosilicate RUB-29 using neutron powder diffraction

High-temperature forms of water-free RUB-29 (Cs14Li42Si72O172) and its Na- and Mg-exchanged modifications were studied by Rietveld analysis with neutron powder diffraction data collected at the instrument SPODI. Their refined structures have helped to explain low and high-frequency relaxation processes resolved in impedance spectra. More importantly, the study showed that, beside the degree of dehydration, the configuration and type of extra-framework cations in the pore system of this topology greatly influence dynamic motions of framework Li cations.

2.2 Casjen Merkel(LMU, Sektion Kristallographie): In situ measurement of lattice deformation and phase content in NiTi shape memory alloys

Shape memory alloys recover their pristine shape after deformation upon heating. We present a neutron powder diffraction study on the stress induced formation of the trigonal R-phase performed at the SPODI diffractometer.

2.3 Alexander Börger(TU Braunschweig): Characterisation of iron-containing Ruddelsden-Popper phases

Ruddelsden-Popper (RP) phases of general composition (ABX3)n·AX (n = 1, 2, ..., ∞) have gained interest especially in the manganate systems due to the effect of colossal magnetoresistance that is exhibited by compounds like $La_{0.8}Sr_{0.2}MnO_3$ and $LaSr_2Mn_2O_7$. Substitution of manganese by iron leads to samples that contain 57Fe suitable for MÃ¶ssbauer spectroscopy. Thus, a series of RP phases of general composition ($LaSrMnFeO_6$)x·SrO (x = 1, 2, ∞) was prepared by sol-gel routes and investigated by a variety of techniques such as room-temperature X-ray diffractometry, scanning electron microcopy combined with EDX, electrical conductivity measurements, temperature-dependent electron paramagnetic resonance spectroscopy, vibrating sample magnetometry, low-temperature Mössbauer spectroscopy, room-temperature FTIR, and Raman spectroscopy. All samples show a magnetic phase transition at lower temperatures, which was elucidated in more detail by neutron diffraction at FRM II at liquid He temperature.

2.4 APPAVOU Marie-Sousai(Forschungszentrum Jülich GmbH - JCNS): Effect of high pressure on the global and internal dynamics of a multimeric protein : case of Haemoglobin studied by quasielastic neutron scattering experiment.

Marie-Sousai Appavou(1), Sebastian Busch(1), Wolfgang Doster(1), Ana GASPAR(2), Tobias Unruh(2)
(1)Technische Universität München, Physik Department E 13, Garching, Germany
(2)Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany

Pressure is a physical parameter which influence is widely spread in Earth. Indeed, micro-organisms like Bacillus Licheniformis can live in Deep Ocean until 10 km and they can sustain pressure of about 1000 bar [1]. Moreover, pressure is more and more used in sterilization and bio-conservation process in food and pharmaceutical industries. A collection of reviews edited by Balny, Masson and Heremans [7] in Biochemica et Biophysica Acta in 2002 brings together a large panel of studies realised with several techniques and on several proteins under pressure [2]. Quasielastic neutron scattering allows to explore at the atomic space scale internal motions of proteins in the pico-second time scale [3,4]. Few neutron scattering studies on biomolecules were performed up to date. The first unfolding study using inelastic neutron scattering was published by Doster et al [5,6]. Other recent studies have been performed by Appavou et al for BPTI [7] and by Di Bari for Trypsin [8]. We would like to present a serie of results as a function of pressure we have obtained recently with the TOFTOF time of flight quasielastic neutron scattering spectrometer (Garching, Germany). We have built a high pressure cell which can sustain a pressure of 2000 bar. The high transmission, due to the aluminium alloy of the cell, allows us to make a quite accurate observation of the influence of pressure on the translational diffusion and the internal dynamics of haemoglobin.

[1] **C. Balny, Bull. Soc. Fr. Biophys. 140 (2003) 10–13.**
[2] **C. Balny, P. Masson, K. Heremans, High pressure effects on biological macromolecules: from structural changes to alteration of cellular processes, Biochim. Biophys. Acta 1595 (2002) 1–402.**
[3] **J.A. McCammon, S.C. Harvey, Dynamics of Proteins and Nucleic Acids, Cambridge University Press, Cambridge, 1988, p. 29.**
[4] **M. Bée, Quasi-Elastic Neutron Scattering, Principles and Applications in Solid State Chemistry, Biology and Materials Science, Adam Hilger, Bristol, 1988.**
[5] **W. Doster and W. Gebhardt, High pressure – unfolding of myoglobin studied by dynamic neutron scattering, Chem. Phys. 292, 2003, 383-389.**
[6] **W. Doster, R. Gebhardt and A. Soper in: Advances in High Pressure Science and Biotechnology II p. 29, Springer 2003, Ed. R. Winter.**
[7] **M.-S. Appavou, G. Gibrat, M.-C. Bellissent-Funel, Influence of pressure on structure and dynamics of bovine pancreatic trypsin inhibitor (BPTI): Small angle and quasi-elastic neutron scattering studies, Biochimica et Biophysica Acta 1764 (2006) 414–423.**
[8] **M. Di Bari, A. Deriu, A. Filabozzi, C. Andreani, A. Di Venere, N. Rosato, Dynamics of trypsin under pressure, Physica B 276–278 (2000) 510–511.**

2.5 Wolfgang Kaltner(Technische Chemie II): 3D Neutronen Tomographie: Zerstörungsfreie Untersuchungen von Hohlkugelkörperstrukturen

Wolfgang Kaltner[1], Klaus Lorenz[2], Andreas Jentys[1], Burkhard Schillinger[2], Johannes A. Lercher[1]
[1]Technische Universität München, Department Chemie, Lehrstuhl II fÃ¼r Technische Chemie, Lichtenbergstraße 4, 85748 Garching, Germany
[2]Technische Universität München, FRM II, Lichtenbergstraße 1, 85748 Garching, Germany

Beschichtete Monolith Strukturen werden schon seit langer Zeit standardmäßig als Katalysatoren zur Autoabgasreinigung eingesetzt. Trägerstrukturen aus gesintertem Edelstahl, die zusätzlich noch Vorteile (z. B. längere Lebensdauer) mit sich bringen, eignen sich dafür ebenso. Mit der Tomographieanlage ANTARES in der Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II, München) wurden Hohlkugelkörperstrukturen mit Neutronen durchstrahlt (Radiographie), um die innere Struktur der Katalysatoren zu untersuchen. Die Ortsauflösung des Neutronendetektors beträgt ca. 100μm. Die 3D-Struktur des Objekts wird aus den unter verschiedenen Winkeln aufgenommenen Radiographien rekonstruiert, um die Verteilung und Größe der Kugeln darzustellen. Bei dieser zerstörungsfreien Messmethode wird fÃ¼r die Separation unterschiedlicher Materialien ein spezifischer Schwächungskoeffizient zugeordnet. Abbildung 1: Struktur Auf der linken Seite in Abbildung 1 wird die berechnete 3D-Struktur der gesamten Hohlkugelkörperstruktur dargestellt. Bei genauer Betrachtung des vergrößerten Ausschnitts (Abb.1 rechts unten) lassen sich sogar Oberflächenstrukturen auf den einzelnen Hohlkugeln feststellen. In Abbildung 1 werden auch Schnitte in axialer, frontaler und sagittaler Richtung durch die Tomographieaufnahme abgebildet. Durch den Schnitt an einer definierten Stelle der Hohlkugelkörperstruktur lassen sich Aussagen Ã¼ber die Homogenität der Verteilung der einzelnen Kugeln in der Struktur an dieser Stelle treffen. Des Weiteren können Wanddichte und Abweichungen vom gewünschten Kugeldurchmesser genauso untersucht werden, wie Deformationen einzelner Kugeln.

2.6 Thomas Finger(Universität zu Köln, II. Physikalisches Institut): Crystal structure and magnetic fluctuations in La(1-x)A(x)CoO(3) (A = Ca, Sr, Ba)

The phase diagram of perovskite cobaltites is closely related to those of the CMR-manganites as they both show ferromagnetism and metallic behaviour at intermediate doping. We have studied the crystal structure of the series with Ca and Ba doping with the SPODI and will discuss the corresponding phase diagrams. Furthermore magnetic excitations were studied by inelastic neutron scattering on PUMA for A = Sr at different doping levels. We report on the magnetism in the ferromagnetic and the spin-glass phase and show the magnon dispersions.

2.7 Richard Mole(FRM II):Inelastic Neutron Scattering From a Distorted Kagome Lattice

The study of ground states and novel excitations in highly frustrated systems is a very active research area. One of the problems faced in the field is preparation of large high purity samples suitable for neutron scattering. Consequently the search for new materials is ongoing. Here we report the inelastic neutron scattering, on a powder sample, of a novel material Mn_3(1,2,4-btc)$_2$. The exchange topology is that of a distorted kagome lattice. Initial analysis of the data shows that to a first approximation the excitation spectrum can be described by that of the conventional kagome lattice.

2.8 Michael Hofmann(FRM II, TU München): Magnetic Phase Transitions and Structures of $Pr_{0.5}Y_{0.5}Mn_2Ge_2$

J.L. Wang[a,b], S.J. Campbell[a], S.X. Dou[b], M. Avdeev[c], A.J. Studer[c], M. Hofmann[d], M Hoelzel[d, e]

[a]School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, The Australian Defence Force Academy, Canberra ACT 2600

[b]Institute for Superconductivity and Electronic Materials, University of Wollongong, Wollongong, NSW 2522

[c]Bragg Institute, ANSTO, Lucas Heights, NSW

[d]Technische Universität München, FRM II, 85747 Garching, Germany

[e] Darmstadt University of Technology, Institute for Materials Science, Petersenstrasse 23, 64287 Darmstadt, Germany

The structural and magnetic properties of $Pr_{0.5}Y_{0.5}Mn_2Ge_2$ have been investigated in detail using X-ray and neutron diffraction and magnetisation measurements (3-570 K). Five different magnetic state regions and four magnetic phase transitions with decreasing temperature have been determined for $Pr_{0.5}Y_{0.5}Mn_2Ge_2$ including a transition from paramagnetism (PM) to intralayer antiferromagnetism (AFI) at around TNintra $\sim$ 375 K which was not reported in a previous dc magnetization study. The second transition from the AFI magnetic structure to a canted spin structure (Fmc) has been detected at TCinter $\sim$340 K. With further decrease in temperature down to below TNinter $\sim$150 K (the third transition), the Fmc magnetic structure gives way to the antiferromagnetic mixed commensurate magnetic structure (AFmc). Finally, the fifth magnetic structure (Fmc+F(Pr)) with the Fmc structure along with additional ordering of the Pr magnetic sublattice is formed when $Pr_{0.5}Y_{0.5}Mn_2Ge_2$ is cooled down below TCPr $\sim$54 K. It was worthy to notice that, compared with the cooling process, the TCPr and TNinter shift to higher temperatures (62 K and 158 K, respectively) when the samples is warming up after zero field cooling process. In addition, TCinter and TCPr are found to increase with applied field while TNinter decreases. Moreover, $Pr_{0.5}Y_{0.5}Mn_2Ge_2$ is found to exhibit strong spontaneous magnetostriction with interplanar antiferromagnetic coupling range.

2.9 Christine M. Papadakis (Physikdepartment E13): TOF neutron reflectometry and GISANS – modern tools for the investigation of thin block copolymer films

Thin films from lamellar diblock copolymers form spontaneously nanostructured surfaces. We have studied the inner film structures of thin films from poly(d-styrene-b-butadiene) using high-resolution TOF neutron reflectometry and grazing-incidence small-angle neutron scattering.

2.10 Ana Gaspar(ZWE FRMII): Time-of-Flight neutron scattering studies on the dynamics of disordered proteins: The case of caseins

Casein proteins belong to the class of natively unfolded proteins. The existence of disordered biologically active proteins questions the assumption that a well-folded 3D-structure is required for functioning and forces a reassessment of the function structure paradigm. A hypothesis generally put forward is that the unstructured nature of these proteins results from the need of a higher flexibility. In order to evaluate if there are significant differences in the dynamics of natively unfolded proteins with regards to that of proteins with a well defined three dimensional structure, a series of dynamic neutron scattering experiments have been carried out at the new neutron facility FRM II in Munich. Here we report the results of neutron time-of-flight measurements performed on the three casein proteins, as well as on myoglobin (a-helices), concanavalin A (b-sheets) and lysozyme (mixed a/b motifs). The possible contribution of neutron backscattering and spin-echo measurements is also addressed.

2.11 Julia Repper (FRM II TUM): Residual stress analysis on IN718 samples at STRESS-SPEC

J. Repper[1,2], M. Hofmann[1], C. Krempaszky[2], W. Petry[1], E. Werner[3]
[1]FRM II, TU München, Lichtenbergstr. 1, D-85747 Garching, Germany
[2]Christian Doppler Laboratorium für Werkstoffmechanik von Hochleistungslegierungen, Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, TU München, Boltzmannstr. 15, D-85747 Garching, Germany
[3]Lehrstuhl fÃ¼r Werkstoffkunde und Werkstoffmechanik, TU München, Boltzmannstr. 15, D-85747 Garching, Germany

Inconel 718 (IN718), a multiphase (e.g. δ-, $\gamma\prime$-, $\gamma\prime\prime$- phase) nickel based superalloy, is frequently used in high temperature jet gas turbines because of its excellent thermal and mechanical properties. Due to changes in microstructure (e.g. precipitates, texture, chemical composition and gradients) during the production process the thermal and mechanical properties of this alloy are strongly affected by the thermo-mechanical treatments during these procedures. In addition to changes in microstructure the different treatments induce residual stresses in

the components. It is well known that residual stresses affect the service lifetime of a component. Neutron diffraction is a powerful tool to characterize residual stresses induced in the components by special sequences of treatments. Different local microstructures within the component can influence the outcome of a diffraction experiment, especially in materials with complex microstructures. This may lead to difficulties in accurate determination of residual stress distributions in these materials. Here we report on the influence of microstructure on residual stress measurements of IN718 samples using neutron diffraction and discuss the ensuing difficulties (e.g. a contradiction with the mechanical equilibrium).

2.12 Fan Yang(Physik-Department E13 TU München): In-situ quasielastic neutron scattering on hydrous silicate melts

The structure and dynamics of water bearing silicate melts is of enormous interests in geoscience as well as technical applications. Several weight percent of water can be stably dissolved in silicate melts at high temperature under high pressure in nature. The macroscopic properties of these melts are highly relevant to many geological processes. Addition of water in silicates has significant influence on their visco-elastic behaviour in the melt but resulting little structure changes in the glassy state . Therefore the investigation of structure and dynamic of theses systems and their links to the macroscopic properties is necessary in order to understand those nature processes. The intrinsic q resolution of quasielastic neutron scattering allows to study the diffusion mechanism in great detail. At the instrument TOFTOF of FRM II a good resolution can be obtained with a large neutron flux, which is ideal to study the dynamics in hydrous silicate melts above their glass transition temperature. High pressure is required simultaneously to suppress water evaporation. In order to measure at high temperature relevant for volcanic processes as well as high pressure samples were measured within a Nb1%Zr pressure cell heated internally with Pt wire under a pressure of 200 MPa using He gas as pressure medium. With an relative long incoming neutron wavelength the Bragg excitation of the cell is avoided. Owing to the fairly small incoherent and absorption cross-section of Nb, an acceptable background from the pressure cell was obtained. Diffusion of water in the sodium trisilicate melt was studied at 5 different temperatures from 850-1250 K under a pressure of 200 MPa. Self-diffusion coefficient of H can be extracted. The observed temperature dependence of the H diffusion coefficient obeys the Arrhenius law with an activation energy of about 0.36 eV. Further investigations based on D_2O samples and other silicate compositions like SiO_2 and Albite are in planning.

2.13 Irena Kucerova(Institute of Chemical Technology Prague): Monitoring of acrylate consolidants penetration through the wood by neutron radiography

Durability of wood depends on exposition conditions and its structure. If wood is stored in suitable conditions, it maintains its appearance and qualities for a long time. On the other hand if wood is exposed to unsuitable conditions it is section to fast deterioration that can even lead to the complete destruction of a wood monument. If wood is already damaged, its consolidation is carried out in order to improve its mechanical properties. For the consolidation to be successful the consolidant solution has to penetrate into the sufficient depth of the wood. Consolidation effects are proportional both to the consolidant amount in the wood and its distribution. That is why it is necessary when studying wood consolidation to use methods that give us information about the flow of polymer solution (consolidant) and its distribution through the wood. The distribution of polymers in the wood structure can be examined, among methods, e.g. by fluorescence and electron microscopy, Raman spectroscopy or indirectly based on changes in the physical and/or mechanical properties of the wood after its impregnation. In contrast with other methods used to detect polymers in wood, neutron radiography provides the possibility to study dynamic processes, i.e. to observe the flow of liquids through wood in real time. Neutron transmission radiography is a nondestructive imaging technique, which monitors the constitution and structure of the examined sample by the transmitted-to-incident neutron radiation intensity ratio. Consolidant solution penetration into the wood bulk depends on the molecular weight of the consolidant, its polarity and stericity, and on its concentration in the solution. Furthermore, penetration of solutions through wood is also affected by the solvent. The transport of solution through wood depends on the penetrability of the particular type and piece of wood, geometry of the artefact and impregnation method applied. Consolidant solutions are applied to the wood by coating with a brush or by spraying; alternatively, the artefact is immersed into the solution under normal, reduced, or increased pressure. Acrylates for consolidation of wooden artifacts are used quite often because of their good resistance both against aging and even minimal shade changes of the impregnated object. However, penetration of polymer solutions into wood depends on their molecular weight and therefore the disadvantage of acrylates is their high relative molecular weight and consequently worse penetration of their solution into wood. Disadvantage of acrylates is their reversal movement to the surface of the object together with an evaporating solvent as well. This contribution describes penetration of acrylic solutions into coniferous and leafy wood which was studied by the neutron radiography. The flow of the solutions through wood progressed due to capillary forces and was studied in the lengthwise direction. The capillary forces are principal of the impregnation by coating with a brush, spraying, immersion under atmospheric pressure and infusion. Studied acrylate solutions are differ in a type of acrylate and its molecular weight, concentration of the solutions and used solvents. The neutron radiography allows us observing of differences in penetrating abilities of acrylic solutions, to monitor moving of the liquid front and gradually increasing amount of solution and its distribution inside the wood sample.

2.14 Sabine Lenser(TU Clausthal): Texture gradient in dissimilar friction welded aluminium

Friction Welding is an innovative solid-state technique which is suitable for similar or dissimilar metals. The base materials are the alloys of steel (316L) and aluminium (AA7020-T6). Particular interest lies on the modification of the local crystallographic texture in the welded and heat affected zone compared to the local texture of the base material. The texture measurements were performed on the neutron diffractometer Stress-Spec using a slit system of 2x2 mm^2. One complete Al-pole figure, i.e. (111), was collected for 12 positions. The results show the texture gradient towards the weld. The texture is changing from deformation texture to fibre texture. This data will help to understand the influence of the friction welding onto the investigated material.

2.15 Dirk Holland-Moritz(Institut für Materialphysik im Weltraum, DLR): Quasielastic neutron scattering on liquid Ni

Materials design from the melt requires the knowledge of diffusion coefficients in melts and the understanding of diffusion mechanisms. Conventional techniques to measure self-diffusion coefficients are hampered by convective fluid flow and possible chemical reactions of the liquids with a container material. We have developed a novel experimental technique that allows the precise measurment of self-diffusion cofficients in metallic melts by combination of the containerless processing technique of electromagnetic levitation with incoherent quasielastic neutron scattering. This allows to access a broad temperature range, including the metastable regime of undercooled melts at temperatures below the melting point. By application of this technique the atomic self motion in liquid Nickel has been studied in a wide temperature range, from 200K above to more than 200K below the melting point. In the whole investigated temperature regime the Ni self diffusion is well described by an Arrhenius law.

2.16 Olaf Schumann(II. Physikalisches Institut): Structure of layered manganites

Manganites with a perowskite structure have attracted strong attention during the past years, mainly because of the discovery of the colossal magneto resistivity effect (CMR) and complex charge, orbital and magnetic ordering phenomena. Because of twinning in the perovskites, precise structural investigations are hampered. We, therefore, investigated the single-layer manganites, which show similar ordering phenomena but only small magneto-resistivity effects. Since these materials are not intrinsically twinned, structure determination can be performed with much higher precision. For the ordered phase of half-doped manganites, two models were proposed, the Zener polaron model with charge ordering on the bonds and the socalled CE-type model with charge and orbital ordering at the

metal-sites leading to two distinct Mn-sites. We present the results of powder and single crystal diffraction studies on $La_{0.5}Sr_{1.5}MnO_4$. From a neutron diffraction experiment performed on the D10 diffractometer we can unambigously discern the two proposed model. The Zener-polaron model does not yield a satisfying description of the observed intensities. Details of the ordered structure in the CE-type model will be discussed. As the D10 data were taken in the orbital ordered phase, but above the Neel-temperature, a second measurement was performed on the Heidi diffractometer, where we collected a number of magnetic reflections.

2.17 Andreas Schlechte(MPI CPfS): As–Se-order of $ZrAs_{1.6}Se_{0.4}$ from Single Crystal Neutron and X-ray Diffraction

Uranium and thorium arsenide selenides display a typical magnetic field independent rise of the electrical resistivity towards lower temperatures ($\leq$20 K) which is explained by a non-magnetic Kondo effect. However, a similar effect has been observed for Zr(As,Se)1.9, which is characterized by a PbFCl type of structure with two sites occupied by As, Se and up to 10 % defects. For discrimination of As and Se we employed single crystal neutron diffraction. The aim of the detailed investigation is to pinpoint the origin of the non-magnetic Kondo behaviour. Large single crystals of ZrAs1.595(3)Se0.393(1) (space group P4/nmm, a = 376.46(1) pm, c = 807.21(2) pm) were grown by Chemical Transport. Structure details were studied with single crystal neutron and X-ray diffraction techniques and the chemical composition determined from wavelength dispersive analysis with X-rays and chemical analyses. Here we present neutron and X-ray diffraction data obtained on a single crystal with composition close to Zr(As,Se)2 and analyse the As–Se-distribution over the two crystallographic non-metal sites.

2.18 Sebastian Stüber(TUM): Quasielastic Neutron Scattering on Refractory Al-Ni melts

In this work quasielastic neutron scattering at time of flight spectrometer Tof-Tof of the FRM II is utilized in order to study atomic dynamics in melts of binary Al-Ni alloys that are the basis of a large variety of high temperature applications. In order to undercool the melts deeply below the melting temperature and to avoid reactions with crucible materials, the liquids are containerlessly processed under high purity conditions by application of the electromagnetic levitation technique. Due to the containerless processing the measured dynamic structure factors are not affected by scattering from a sample container such that the quasielastic neutron scattering measurements were possible also at large momentum transfer. From the measured dynamic structure factors Ni self-diffusion coefficients are determined as a function of alloy composition and temperature. At constant temperature, the Ni self diffusivity is constant within a wide compositional range.

2.19 Jan Perlich(TUM, Physik-Department, LS E13): Solvent content in thin spin-coated polymer films

The detection of remaining solvent in thin polymer films is of importance due to its effect on chain mobility and film homogeneity. Moreover, it gives an estimate on possible aging effects caused by the reduction of the solvent content, which typically yield an increased brittleness. In the present investigation, we focus on a well controlled model system, which consists of protonated polystyrene (PS) with different molecular weights, spin-coated out of protonated or deuterated solvent onto silicon wafer substrates. Directly after spin-coating the thin PS films were investigated with neutron reflectivity (NR) at the MIRA instrument of FRM-II. A narrow qz range around the critical edge was probed with high resolution. Due to the high sensitivity of the position of the critical edge on the ratio of protonated PS and deuterated solvent, the exact position of the critical edge enables to determine the solvent content. In addition to the deuterated solvent samples, samples with thin PS films spin-coated out of protonated solvent were also prepared for a direct comparison of the different sample types. Two different key parameters which influence the solvent content: the molecular weight of PS and the film thickness in the range of 10 nm to 100 nm were investigated. A direct comparison indicates a clear distinction between thin films prepared of PS dissolved in protonated or deuterated solvent. This directly transforms into the amount of solvent remaining in the polymer film. Depending on the molecular weight of PS, the shift of the critical edge is pronounced to a greater or lesser extent, but clearly visible. The actual sample preparation conditions are of importance and affect the amount of solvent inside the PS films.

2.20 Gernot Goll (Physikalisches Institut Universität Karlsruhe): Inelastic Neutron Scattering on the antiferromagnetic Half-Heusler Alloy CeBiPt *

CeBiPt is a semimetal with a rather low charge carrier concentration n=$7.7{\cdot}10^{17}$,cm^{-3}. Below $T_{mN} \approx 1$,K antiferromagnetic order occurres as evidenced by sharp maxima in the thermodynamic properties. Neutron diffraction experiments have revealed an AF-type I structure with a propagation vector $au = (1\ 0\ 0)$ and moments also along $[1\ 0\ 0]$. The ordered moment $\mu \approx 0.6\mu_B$ is much lower than the effective moment determined from the Curie-Weiss behavior of the susceptibility at higher T. Crystal-electric field (CEF) splitting of the Ce^{3+} level might be one origin of a lowered ordered moment. We performed inelastic neutron scattering experiments on TOFTOF at the FRM-II with energy of the incident neutrons $E_i = 2.7$, 5.7, and 16.9,meV and on PANDA with $E_i = 5.6$,meV at $.8 < T < 50$,K. We found only one CEF excitation at $\hbar\omega \approx 9.5$,meV at $T = 2$,K in line with previous measurements on SV29 at FRJ-2 with fixed $E_i = 30$,meV. This excitation has been identified with the transition between a Γ_7 doublet and a Γ_8 quartet state. No further inelastic excitations have been observed except for a quasielastic contribution which increases in width with increasing temperature.

* **in collaboration with: O. Stockert, T. Unruh, P. Link, K. Shigetoh, T. Takabatake**

2.21 Dmitry Lebedev (Petersburg Nuclear Physics Institute): Structure of nucleoprotein complexes: neutron scattering studies

Investigation of two distinct types of the biological systems that represent nucleoprotein complexes of different levels of organization are carried out in Division of Molecular and Radiation Biophysics of Petersburg Nuclear Physics Institute RAS. Bacterial RecA proteins are the key enzymes in the process of homologous recombination. Large-scale filament structure of the proteins form nucleoprotein complexes with DNA to facilitate the exchange of homologous strands between single- and double-stranded DNA. The structure and dynamics of these complexes were studied by SANS on YuMO (JINR, Russia), KWS-1, KWS-2 (IFF, Germany) and D-11 spectrometers (ILL, France) (Lebedev et al., FEBS Letters 2003, 537: 182-186; Petukhov et al., Proteins 2006, 65: 296-304; Lebedev et al., Biophizika, in print). Currently the study is focused on the molecular basis of the flexibility of the nucleoprotein filaments formed by homologous recombinases with the use of different wild-type and mutant RecA proteins being expressed and purified in the laboratories of our Institute. The other type of nucleoprotein complexes being investigated in our laboratories is chromatin fiber. In intact nuclei of cells of higher organisms chromatin exhibits highly hierarchical structure that serves on one hand very dense packing of DNA within cell nucleus, and on the other hand high accessibility of genome to the replication, repair and translation machinery. Started by using the tandem of KWS-2 and KWS-3 spectrometers in Juelich and followed by D-11 experiments, we obtained the data on hierarchy of the native chromatin on wide range of scales, from nucleosome structure to the nucleic compartments (Lebedev et al., Kristallografiya, in print) in different cell types. Currently preparative procedures have been developed in PNPI to obtain intact isolated nuclei of a number of cultured cell lines, including human cancer cell lines, in quantities required for SANS experiments. Use of KWS-2 and KWS-3 would allow comparative study of the chromatin structure in intact nuclei of normal and cancer cells.

2.22 Ezzeldin Metwalli(TUM, Physik Dept. E13): Structural investigation of diblock copolymer thin films using TOF-GISANS at REFSANS

Polymer thin films of polystyrene-block-polyisoprene, P(S-b-I), diblock copolymer were spanned over a wide q range in a single measurement using wavelength from 2-21 Åin a time-of-flight mode GISANS at REFSANS. The TOF-GISANS results indicated that P(S-b-I) diblock copolymer has lamella structures parallel to the surface with lamella thickness of 49 nm. The results are compared with the GISANS data obtained on D22 beamline at ILL and idicated the advantages of using multiple wavelengths which provide multiple scattering effects. The study aimes to investigate the surface constraint on self-assembled polymer and the effect of modification of interfaces to direct the formation of more complex structures.

2.23 Tarik Mehaddene (Physik-Department E13, TU München): Dynamical properties of magnetic shape memory alloys from inelastic neutron scattering

T. Mehaddene[1], J. Neuhaus[2], W. Petry[1,2]
[1] Physik-Department E13, TU München
[2] Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), TU München

Magnetic shape memory alloys belong to a class of smart materials able to recover large magnetic field induced strains under moderate fields. Necessary for the occurence of this effect is a structural transformation from a high temperature phase (austenite) to a low temperature phase (martensite). Inelastic neutron scattering on single crystals is a powerful technique to investigate the dynamical precursors of such transformations. We report on phonon measurements along the $[110]$ direction and their temperature dependence in different Ni-based Heusler alloys. The measurements have been performed in both austenitic and martensitic phases. Fundamental difference are observed in the phonon dispersions of the five-layered (5M) and seven-leyred (7M) modulated martensitic phases of Ni_2MnGa.

2.24 Hans Boysen (LMU, Kristallographie):Kristallstruktur und Sauerstoffbeweglichkeit in Mayenit (Ca12Al14O33): Hochtemperaturuntersuchungen mit Neutronen-Pulver-Diffraktion

H. Boysen[1], I. Kaiser-Bischoff[1], M Lerch[2], M. Hölzel[3], A. Senyshyn[3]
[1]Department f. Geo. und Umweltwissenschaften, Sektion Kristallographie, LMU, Theresienstr. 41, 80333 München
[2]Institut für Chemie, TU Berlin, Straße des 17. Juni 135, 10623 Berlin
[3]TU Darmstadt/FRM II, TU München, Lichtenbergstr. 1, 85747 Garching

Mayenit (Ca12Al14O33) ist ein schneller Sauerstoffionenleiter [1], der aus einem Calciumaluminat-Gerüst besteht, in das 32 der 33 Sauerstoffionen fest eingebunden sind. Das 33. Sauerstoffion ist statistisch über 1/6 der Käfige in der Struktur verteilt. Es kann gegen andere Ionen (z.B. F-, OH-, sogar Elektronen) ausgetauscht werden. Kürzlich konnten auch N3- Anionen eingebaut werden. Die Synthese gelingt durch Festkörperreaktion aus Al_2O_3 und $CaCO_3$ mit mehrmaligem Aufheizen auf etwa 1300°C und anschließendem Vermahlen. Am Gerät SPODI/FRM2 wurden Neutronen-Pulverbeugungs-Untersuchungen von Raumtemperatur bis 1050°C durchgeführt. Das 'freie' O-Anion konnte eindeutig über Differenz-Fourier Methoden lokalisiert werden. Bei Raumtemperatur wurde eine Überbesetzung entsprechend Ca12Al14O33.53 gefunden, was mit dem Einbau von O-, O2-, O22- und OH- Anionen erklärt wird. Oberhalb von 700°C wird die ideale stöchiometrische Zusammensetzung erreicht. Auf Grund der erhaltenen Ergebnisse muß die Struktur (im Gegensatz zur Literatur!) als stark fehlgeordnet beschrieben werden, bestehend aus einem Gerüst aus 8er-Ringen von AlO_4-Tetraedern, in das sowohl das 'freie' O als auch Ca statistisch eingebettet sind, wobei letztere

eng aneinander gebunden bleiben [2]. Bei hohen Temperaturen sind die Dichten des 'freien' O extrem stark ausgeschmiert, was mit der hohen Ionenleitfähigkeit in Einklang ist. Weitere Ergebnisse zeigen, dass die Diffusion über einen Austausch mit dem Gerüst-Sauerstoff stattfindet, in Übereinstimmung mit kürzlichen molekulardynamischen und ab initio Rechnungen [3]. Die Arbeiten werden im Rahmen des SPP 1136 durch die DFG (BO 1199/2-3, LE 781/10-4) unterstützt.

[1] **Lacerda, M., Irvine, J. T. S., Glasser, F. P., West, A. R.: Nature (1988), 332(6164), 525-6**

[2] **Boysen H., Lerch M., Stys A., Senyshyn A.: Acta Cryst. B63 (2007) 675-682**

[3] **Sushko, P.V., Shluger, A.L., Hayashi, K., Hirano, M. & Hosono, H.: Phys. Rev. (2006) B73, 014101-1-10**

2.25 Robert Metzke(Group for Computational Mechanics): Neutron Tomography of Rat Lungs

Mechanical ventilation is the most important life saving therapy for respiratory failure. However, due to mechanical stress that the ventilator imposes to the patients respiratory system with every breath, further lung damage may occur as severe side effect of mechanical ventilation itself. In order to minimize the risk of the so-called *ventilator-induced lung injury*, we need to understand the link between the ventilator settings and the energy transfer to the lung tissue. To do so, an extended mathematical model to describe the dynamic mechanics of respiration, based on animal experiments and detailed finite element simulations, is developed. The model will approach the problem from two different scales. On the one hand the dynamics of the coupled flow-structural mechanics problem with focus on non-linear alveolar and lower airways mechanics shall be investigated. Through the combination with a more clinical model of global mechanical behaviour we want to be able to predict the individual patients risk for lung damage and find the best individual ventilator settings based on bedside measurements. For the detailed simulation of lower airways the derivation of the geometries of these structures is challenging. Here we show that neutron tomography is able to image the airway structure of rat lungs up to the 7th generation of a complete rat lung. The imaging up to this high number of generation together with the fact that not only certain parts of the lung a imaged, but the complete structure, are a excellent basis for large-scale fluid structure simulations in order to better understand the behavior of the lung under mechanical ventilation.

2.26 Ahmed Esmail(nuclear power plants authority): N-ray versus X-ray for void detection in materials

Neutron radiography (NR) has already proved itself as a successful tool of nondestructive testing (NDT) in many applications. It is considered to be complement (and alternative in some cases) to conventional X-ray radiography. This is because neutrons have unique scattering and absorption properties for the study of internal structures and hidden flaws in non-destructive testing of materials. Thus, the attenuation of neutrons is a function of the nucleus rather than the

density of electrons in a material as in the case of X-rays radiography. The MCNP calculations were used to determine the capability of both neutron radiography and X-ray radiography for porosity inspection in iron, ceramic and polyethylene. Experiment was applied in order to support/validate theoretical works. Both theoretical and experimental results showed that X-rays are superior to N-rays for detection of voids in iron and ceramics while neutrons are preferred in case of PE.

2.27 Thomas Bücherl (RCM TUM): Inspection of a Gear Box by Fission Neutron Radiography

T. Bücherl[1], Ch. Lierse v. Gostomski[1], H. Erntl[1], B. Schillinger[2]
[1]Institut und Lehrstuhl für Radiochemie, Technische Universität München, Walther-Meißner-Str. 3, 85748 Garching, Germany
[2] Forschungsneutronenquelle Heinz Maier-Leibnitz FRM II, Lichtenbergstr. 1, 85748 Garching, Germany

Nowadays, non-destructive testing has become an essential tool in quality control and quality assurance for development and production of not only technical goods. While X-ray radiography is very often the preferred technique for this purpose, it sometimes fails in giving the required information due to simple physical reasons like too small penetration power of the X-rays or limited contrast for similar materials. Here, fission neutron radiography can step into the gap giving complementary information as the interaction of fission neutrons with matter is completely different to that using X-rays. This is illustrated by an example out of praxis. For a gear box the filling height of the oil had to be determined non-destructively. Radiographs, applying X-rays, gamma-rays, thermal neutrons and fission neutrons, respectively, are presented and compared.

2.28 Thomas Bücherl (RCM TUM): Fission Neutron Radiography and Tomography of Wood

T. Bücherl[1], Ch. Lierse v. Gostomski[1], E. Kutlar[1], K. Osterloh[2], Ch. Rädl[2]
[1]Institut und Lehrstuhl für Radiochemie, Technische Universität München, Walther-Meißner-Str. 3, 85748 Garching, Germany
[2]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany.

As a naturally grown material, wood has been used for many purposes during the whole history of mankind, either as consumable or for manufacturing items of the daily life. Often it is used for constructions where everyone relies on its integrity, e.g. bridges, houses and ships. This integrity might be diminished by biological or mechanical degradation. The recognition of such defects in due time and at an acceptable reliability level is therefore of prime importance. The deepest non-destructive insight into the inner structures of wooden objects is

given by computerized tomography. In contrast to X-ray and gamma-ray tomography fission neutrons are capable to visualize the internal distribution of moisture. This is of concern, particularly, in lumber or in girders, since this can make them prone to rot. In a first series of measurements by means of fission neutron radiography and tomography at the NECTAR facility at FRM-II, different wooden samples have been investigated non-destructively demonstrating the applicability of these methods.

3 Poster Instrumentation

3.1 Bert Nickel(LMU): A sample environment for biological interfaces

We have developed a microfluidic neutron sample cell for neutron reflectivity experiments. The cell allows for complementays in-situ studies of biological interfaces by reflectometry and fluorescence microscopy, thus structural and dynamical interface properties can be compared. We have used this cell to study membrane associated proteins such as Annexin 2. Results from PSI(Amor) and Refsans(FRM II) are presented.

3.2 Jürgen Peters, Sample environment at FRM II

The central sample environment group at FRM II provides a wide range of different devices covering environmental parameters like high and low temperature, magnetic field, high pressure etc. The standard device for low temperatures is our in-house developed cryogen free sample tube cryostat CCR providing a temperature range from about 700 K to 3.2 K. Furthermore the CCR gives the base for inserts like continuous ^{3}He-or dilution units, extending temperatures to 400mK and 50mK respectively. Beside the CCR, several GM type closed cycle refrigerators are available, some of them with special adoption to instrument demands like operation in goniometers. High temperature experiments can be performed using our high temperature furnace HTF providing temperatures up to 2200 K or using a very compact infrared furnace. This device allows for experiments up 1400 K in different gas atmospheres and small samples. At the spectrometer TOFTOF a *Bio-Furnace* for moderate temperatures ranging from 240K to 400K is available. Magnetic fields up to 15 T allow for studies of magnetic properties. A cryogen free 7.5 T magnet with a 100 mm room temperature bore is available. This allows for the combination of additional environments like low or high temperatures, pressure etc. The 15T magnet is dedicated to the spectrometer PANDA. A dilution unit provides temperature down to 100 mK. High pressure experiments can be performed using a gas high pressure device up to 1 GPa. In collaboration with the Bayerisches Geoinstitut a Dual Anvil Cell is available for small samples. Furthermore we develop and improve our systems continuously. Current developments are e.g. a high pressure cryostat, electrostatic levitation e and a furnace for a tension test rig.

3.3 Klaudia Hradil(Inst. f. Physikal. Chemie, Universität Göttingen): Real time spectroscopy at PUMA

K. Hradil[a], J. Leist[a], F. Güthoff[a], R. A. Mole[b] and G. Eckold[a]
[a] **Institut für Physiaklische Chemie, Universität Göttingen, D-37077 Göttingen**
[b] **Neutronenforschungsquelle Heinz Maier-Leibnitz, Technische Universität München, D-85747 Garching**

Inelastic neutron scattering technique provides information about the microscopic dynamics of solids. Investigations on a real time scale within external fields (temperature, pressure, magnetic/electrical fields) would yield the microscopic information of relaxation processes (phase transitions, domain order/disorder processes, decomposition processes). Conventional inelastic neutron scattering technique is due to the low intensity of the investigated excitations and therefore the relatively long measuring times beyond the scope for real-time experiments in timescales which are of interest. Eckold [1] introduced a method to combine real time resolution together with inelastic neutron scattering by a stroboscopic measuring technique. By cycling of the sample in an external field, the scattered intensity is not only detected as a function of momentum and energy transfer but also sorted within time channels. The reversibility of the processes is a necessary condition for the application of the technique. This technique was recently implemented within the spectrometer electronics of the triple axis spectrometer PUMA at FRM II and can provide the possibility to analyze excitations within relaxation processes on a timescale down to microseconds. Beside introducing the technique and possibilities for performing experiments first experiments applying electrical fields for the study of ferroelectrics or cycling of temperature to follow decomposition processes will introduced.
[1] **G. Eckold "Time-resolved triple axis spectroscopy - a new method for real-time neutron scattering" Nucl.Instr. Methods A289, 221 (1990)**

3.4 Anatoliy Senyshyn(Darmstadt University of Technology): Structure powder diffractometer SPODI

M. Hoelzel, A. Senyshyn, H. Boysen, H. Fuess

The Structure Powder Diffractometer SPODI at FRM II is a product of collaboration between Darmstadt University of Technology, Ludwig-Maximilians University Munich and University of GÃ¶ttingen. The SPODI was designed as a high resolution powder diffractometer and it is mostly suited for nuclear and magnetic structural determination/refinement, studies on phase transformations and evolution of the microstructure at various experimental conditions. The Structure Powder Diffractometer SPODI is in user service at research reactor FRM II since June 2005. During the time of operation more than 70 user experiments were successfully carried out for more than 45 proposers all over the world. This contribution gives an overview on specifications, available sample environment, recent developments and plans for future together with selected examples of measurements.

3.5 Sergey Masalovich(FRM II): HELIOS - polarized ^{3}He gas for neutron instrumentation

Neutron spin filters based on a dense hyperpolarized ^{3}He gas may compete in polarization efficiency with common devices such as magnetized single crystals or supermirrors. Although these other methods are rather simple in operation, their applications are strongly limited by the acceptable neutron energy and the allowed range of scattering angles. By contrast, broadband neutron spin filters can be built to a predetermined size and shape in such a way that they will meet just about all practical needs.

3.6 Vladimir Hutanu (RWTH Aachen): POLI-HEiDi project: New Polarised Hot Neutron Diffractometer for Magnetic Structures at FRM II

Vladimir Hutanu[1,2], Martin Meven[2], Gernot Heger[1]
[1] **Institut for Crystallography RWTH Aachen, Jägerstr. 17-19, 52056 Aachen Germany**
[2] **TU München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz FRM II, Lichtenbergstr. 1, 85747 Garching Germany**

Since the end of 2004, the Institute for Crystallography at RWTH Aachen started the project (supported by German Federal Ministry of Education and Science BMBF) to extend the already existing new single crystal diffractometer HEiDi at FRM-II for a polarised neutron option to enable detailed investigations on the magnetic order of single crystals. The evaluation of the problems by implementing the polarised neutron option on the existing instrument lead to the decision to build a parallel instrument especially designed for this purpose, called POLI-HEiDi (Polarisation Investigator- HEiDi). Both options, zero-field 3D (spherical) polarisation analysis with Cryopad and MuPAD polarimeters as well high magnetic field flipping ratio method for magnetisation density maps measurements should be available at the new instrument. Taking into account the advantages of the polarised 3He spin filters for increasing of the polarised neutrons flux, especially for the hot neutrons and benefit by available at FRM II high capacity polarised ^{3}He production facility HELIOS the ^{3}He NSFC (Neutron Spin Filter Cells) have been choose as a polarisation method. The results of the first experiments with ^{3}He NSFC performed recently at the existing HEiDi diffractometer are discussed. Design and construction of the new instrument are presented. A number of components for the new polarised diffractometer have been developed, produced and successfully tested.

3.7 Janosch Major (MPI Metallforschung): N-REX$^+$ – the Neutron/X-ray Contrast Reflectometer for Materials Science

A. Rühm, J. Franke, M. Major, M. Nülle, J. Major, H. Dosch
Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

The neutron reflectometer with add-on X-ray option, N-REX$^+$, is a so-called "tanzboden instrument". The facility uses neutrons of the FRM II cold source which are transported to the instrument site at the neutron-guide hall by the neutron guide NL1 and extracted by a focused array of HOPG (highly oriented pyrolytic graphite) monochromator crystals. The neutron wavelength can be adjusted between 2 Å and 6 Å, the energy width is approximately 1-2%. The neutron detector is a 2-dimensional wire chamber of a size of 190 mm $\times$ 190 mm, its spatial resolution is approximately 2 mm.

The operation modes of the instrument includes conventional neutron reflectometry and off-specular scattering, reflectivity and off-specular scattering of polarized neutrons with wide-angle spin analysis of the scattered neutrons, X-ray reflectometry, or spin-echo resolved grazing incidence scattering (SERGIS).

The sample can be solid, soft matter, or liquid (their surfaces or buried interfaces, magnetic or non-magnetic layers or multilayers). The basic sample position is horizontal, but experiments on vertical samples are possible, too. Experiments on samples with free liquid surfaces are also feasible.

The sample environment can be amongst others air, vacuum, controlled atmosphere of inert or slightly reactive gases or vapours at temperatures up to 300 $^\circ$C, low temperatures down to 2.5 K, magnetic fields up to 7.5 T, or a silicon cell for thin liquid samples.

3.8 Yixi Su (JCNS) DNS - A new polarized time-of-flight spectrometer at FRM II

DNS, a versatile multi-detector time-of-flight spectrometer with full polarization analysis, is currently being constructed by the JCNS outstation at FRM-II. Very recently, the fist neutrons and intense polarized beam have been achieved at DNS. The current status and the upcoming construction plan will be given in details. DNS is highly suitable for the investigations of magnetic, lattice and polaronic correlations in various length and time scales from many correlated electron materials and frustrated magnets. The scientific prospects will be presented.

3.9 Astrid Schneidewind (TU Dresden): Cold three-axis spectrometry on PANDA.

We present characteristics, performance and examplary results of the cold three-axis spectrometer PANDA.

3.10 Martin Meven (FRM II, TU München): Structural Investigations with the hot Single Crystal Diffractometer HEiDi

The single crystal diffractometer HEiDi at the research neutron source Heinz Maier-Leibnitz (FRM II) was designed to cover a broad range of scientific applications in crystal structure analysis by using the high flux of fast neutrons from the hot source of the FRM-II. This hot source consists of a graphite cylinder in front of the beam line of HEiDi which is heated up to about 2300 Kelvin by the radiation of the reactor core. Therefore, the thermal neutron spectrum becomes moderated to a hot one with a maximum at about 0.5 Åand a significant gain factor of neutron flux around 8 at this wavelength. Neutron diffraction experiments at HEiDi use the advantage of the independence of the nuclear scattering lengths b from the Q value ($Q = sin\theta/\lambda$). Therefore, the intensities of Bragg reflections at large Q values become strong enough to reveal structural details. The enlargement of the visible reciprocal space allows very accurate determinations of nuclear positions in single crystals, e.g. in the context of H-bonds, as well as very detailed investigations on other structural properties like anisotropic mean square displacements and vacancies which are of interest in reference to static or dynamic disorder effects and phase transitions. In addition, the difference between the Q-dependences of the magnetic and the nuclear cross sections of neutrons can be used to determine the magnetic and the nuclear order in a crystal separately. Further advantages of short neutron wavelengths at HEiDi (1.4 Ådown to 0.3 Å) are the significant reduction of absorption effects in compounds with highly absorbing elements (e.g. Sm, Gd) and the reduction of extinction effects. The sample environment of HEiDi covers a broad temperature range between 2 Kelvin and 1100 Kelvin which gives the opportunity to detailed investigations of structural and magnetic phase transitions with neutrons.

3.11 Reinhard Kampmann (GKSS Research Centre): Performance of the Horizontal Reflectometer REFSANS at FRM II

The reflectometer REFSANS allows to perform comprehensive analyses of vertical and lateral surface and interface structures by means of specular and off-specular neutron reflectivity as well as small-angle neutron scattering at grazing incidence (GISANS). All measurements can be performed on the air-water interface (horizontally aligned sample). REFSANS has successfully been put into operation, its performance is highlighted by recently obtained experimental results.

3.12 Ulf Garbe (GKSS) New Instrument Concepts for the Materials Science Diffractometer STRESS-SPEC at FRM II

[1]Ulf Garbe, [2]Joana Rebelo-Kornmeier, [3]Andreas Ostermann, [3]Michael Hofmann
[1] GKSS Forschungszentrum, Max-Planck-Str. 1, D-21502 Geesthacht
[2] Hahn-Meitner-Institut, Glienickerstr. 100, D-14109 Berlin
[3] FRM-II, TU München, lichtenbergstr. 1, D-85747 Garching

The Materials Science Diffractometer STRESS-SPEC at the German neutron source FRM-II is designed to be equally applied to texture and residual stress analysis. First experimental results using slit based optics show that even with small gauge volumes down to 1x1x1 mm^3 residual stress and texture analysis is easily feasible on STRESS-SPEC. However, with measurement positions deeply embedded inside components and for local texture applications it is important to further optimise neutron flux and sample positioning. In the first part (optimisation of neutron flux) we will present a comparison between Monte Carlo simulations and experimental measurements where a prototype parabolic focussing guide replaced the primary slit. The major advantage of parabolic focusing is that the flux maximum occurs not at the exit of the tube. It occurs at the focal point that can be several centimetres away from the tube end. The experimental results were in good agreement with the simulations. Both an improved definition of a small gauge volume even deep within the sample material and a substantial flux increase at the sample position were observed when simulations were done for an optimised parabolic guide for Stress-Spec. Furthermore we will show the advantages of using a new robotic system to enhance the capabilities of STRESS-SPEC for 3-D residual stress and local texture analysis. This system will be installed in addition to our existing conventional goniometers (Eulerian cradles) for 3-D strain and texture analysis and is superior with respect to feasible sample size, speed and translation range.

3.13 Burkhard Schillinger (FRM II): ANTARES

The ANTARES neutron imaging facility for cold neutrons offers a variety of imaging methods with neutrons. As an image says more than a thousand words, the poster shows several typical applications of neutron imaging, many of them in direct comparison to X-ray imaging. The typical properties and possibilities are illustrated in many examples, an additional poster shows all the components of the ANTARES facility.

3.14 Robert Georgii (FRM II TUM): MIRA at the FRM II

Robert Georgii, Peter Böni, Reinhard Schwikowski, Sebastian Mühlbauer, and Marc Janoschek

MIRA is a versatile instrument for very cold neutrons (VCN) using neutrons with a wavelength $\geq$ 8Å. The flux at the sample position is $5 \cdot 10^5 neutrons/(cm^2 s)$ unpolarized. It is situated at the cold neutron guide NL6b in the neutron guide hall of the FRM II. As the instrument set-up can be changed quickly, MIRA is ideally suited as a testing platform for realizing new instrumental set-ups and ideas. In particular, MIRA is unique in its possibilities of combining different neutron scattering methods as:

- **Polarized or non-polarized reflectometry.**
- **Spherical Polarimetry**
- **Polarized or non-polarized small angle scattering (SANS).**
- **Classical NRSE (Neutron Resonance Spin Echo) set-up as well as using the MIEZE principle.**

A polarizing multilayer monochromator was taken into operation recently. This allows now full polarization analysis, 3D-polarimetry and MIEZE measurements. Selected experiments using these options together with an outlook to the current upgrade of the instrument will be presented here.

3.15 Lhab Abdel-Latif (Nuclear Research Center): The Polarized Neutron Diffraction at Low Power Reactor

The present work deals with the calculations of the polarized neutron diffraction option for the Cairo Fourier Diffractometer Facility CFDF. The CFDF is based on the reverse time of flight RTOF diffraction method using Fourier chopper. The Neutron flux incident on the sample is 10^6 neutrons·cm^{-2}·s^{-1} in the case of non-polarized neutron diffraction, (in the present time). The polarized neutron PN possibility will decrease the intensity incident on the sample $\sim 2x10^5$ neutrons.cm^{-2}.s^{-1} with resolution of $5x10^{-3}$. The PN option enable studying the magnetic structure and spin density of the magnetic materials besides suppressing the incoherent contributions in the diffraction pattern

3.16 Tobias Unruh (FRM II): Quasielastic and inelastic neutron scattering at the time-of-flight spectrometer TOFTOF

C.Smuda, S.Busch, J.Ringe, J.Neuhaus, W.Petry, T.Unruh
Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

The multi-chopper time-of-flight spectrometer TOFTOF at the cold neutron source of the FRM II is in routine operation since July 2005. Its excellent signal-to-noise ratio, high flux, and wide-tunable resolution offer new possibilities in quasi-elastic and inelastic neutron scattering. In this contribution, the performance of the spectrometer is demonstrated using examples taken from the in-house research program 'Neutron Spectroscopy for Applied Pharmaceutical Research'. Complex colloidal aqueous emulsions designed for drug delivery are investigated regarding diffusive and internal motions of both drug carriers (lipid-like substances) and emulsifiers (in particular phospholipids). The results from high resolution, inelastic and quasi-elastic measurements will be presented and were selected in order to demonstrate different features of the TOFTOF spectrometer.

Table 3.1: List of participants

name	affiliation
Ahmed Esmail	nuclear power plants authority
Alexander Bürger	TU Braunschweig
Alexander Diethert	Physik Department, E13
Alexander Ioffe	JCNS
Ana Gaspar	ZWE FRMII
Anatoliy Senyshyn	Darmstadt University of Technology
Andreas Houben	Institut für Anorganische Chemie
Andreas Laumann	Departmant für Geo- und Umweltwissenschaften, LMU
Andreas Ostermann	Forschungsneutronenquelle Heinz Maier-Leibnitz
Andreas Schlechte	MPI CPfS
Angela Vasilescu	Horia Hulubei Nat.Inst. for Physics&Nucl.Engineering
Anja Ines Pommrich	Institute of Materials Physics in Space
Ann Falk	MPI für Polymerforschung
Annette Spiekermann	Anorganische Chemie Neue Materialien
APPAVOU Marie-Sousai	Forschungszentrum Juelich GmbH - JCNS
Astrid Schneidewind	TU Dresden
Bakari Magoma	twentyfoursevenlimited
Bert Nickel	LMU
Burkhard Schillinger	FRM II
Casjen Merkel	LMU, Sektion Kristallographie
Christian Pfleiderer	Technische Universität München
Christine M. Papadakis	Physikdepartment E13
Conradin Kraemer	ETHZ&PSI
Daniel Senff	II. Physikalisches Institut, Universität zu Köln
Dirk Holland-Moritz	Institut für Materialphysik im Weltraum
Dirk Visser	FRM II
Dmitry Lebedev	Petersburg Nuclear Physics Institute
Ezzeldin Metwalli	TUM Physics Department
Fabian Schmitz	TU Braunschweig, Institut für Werkstoffe
Fan Yang	Physik-Department E13 TU München
Feng Liang	FRM II
Florian Henkel	TUM, FRM II
Gernot Goll	Physikalisches Institut Universität Karlsruhe
Gunar Kaune	TU München, Physik-Department LS E13
Hans Boysen	LMU, Kristallographie
Hans-Joachim Gudladt	Inst. für Werkstoffkunde, LRT5
Harald Hilbig	Centrum Baustoffe und Materialprüfung TU München
Helena Hartmann	Institut für Materialphysik im Weltraum
Helmut Ehrenberg	IFW Dresden
Ihab Abdel-Latif	Nuclear Research Center
Irena Kucerova	Institute of Chemical Technology Prague
Irina Shtangeeva	St. Petersburg University
Isiaka Ngoroki	twentyfoursevenlimited
Jan Perlich	TUM, Physik-Department, LS E13

Table 3.1: List of participants (continuation)

name	affiliation
Janos Major	Max-Planck-Institut für Metallforschung Stuttgart
Joachim Wuttke	JCNS
Jörgen Franke	MPI-MF
Jörg Schefer	ETH Zürich & Paul Scherrer Institut
Jürgen Neuhaus	FRM II, Technische Universität München
Jürgen Peters	ZWE FRM II
Jean-Francois Moulin	TUM E13
Jimei Guo	Institut für Radiochemie
Joachim Baumann	Siemens CT
Julia Repper	FRM II
Karl Zeitelhack	FRM II
Klaudia Hradil	Inst. f. Physikal. Chemie, Universität Göttingen
Klaus Lorenz	FRM II
Klaus Schreckenbach	Physik Department E21, TU München
Krunoslav Prsa	Paul Scherrer Institute
Markus Hölzel	TU Darmstadt
Markus Ruhstorfer	iwb (TU München)
Martin Meven	FRM II, TU München
Marton Major	MPI für Metallforschung
Mathias Dörr	TU Dresden, Institut für Festkörperphysik
Michael Hofmann	FRM-II, TU Munich
Mohamed Mohamed	TU-Darmstadt
Olaf Schumann	II. Physikalisches Institut
Oliver Senftleben	Institut für Physik (EIT9)
Peter Böni	Fakultät für Physik E21
Peter Müller-Buschbaum	TU München Physik Department E13
Rainer Niewa	
Ralph Gilles	FRM II, TU München
Raquel Munoz Horta	Institut für Physik - Universität Mainz
Regina Klein	Institut for Physikalische und Theoretische Chemie
Reinhard Kampmann	GKSS Research Centre
Richard Mole	FRM II
Robert Metzke	Group for Computational Mechanics
Robert Wimpory	Hahn Meitner Institut
Robin Beddoe	Centrum Baustoffe und Materialprüfung
Rupert Gebhard	Archaeologische Staatssammlung
Sabine Lenser	TU Clausthal
Sarah Dunsiger	Physics Department E21
Saskia Bernstein	Departmant für Geo- und Umweltwissenschaften, LMU
Sebastian Stüber	TUM
Sergey Masalovich	FRM II
Shinya Tsukada	University of Tsukuba
Sohyun Park	LMU München, Geowissenschaften
Tarik Mehaddene	Physik-Department E13, TU München

Table 3.1: List of participants (continuation)

name	affiliation
Tobias Unruh	FRM II, TUM
Thomas Bücherl	Institut für Radiochemie
Thomas Fehr	Dept. Geo- & Umweltwissenschaften
Thomas Finger	Universität zu Köln, II. Physikalisches Institut
Thomas Gutberlet	JCNS
Ulf Garbe	GKSS
Volker Körstgens	TUM Physikdepartment E13
Wilhelm Klein	FRM II
Wolfgang Kaltner	Technische Chemie II
Wolfram Lorenz	IFW Dresden
Yixi Su	JCNS