FRM II news

Nº 1

YANL - Yet Another News Letter ?

Dear colleagues and friends,

About three years ago we started our routine operation of the reactor in May 2005, while still struggling with the commissioning of the first instruments. In the mean time we have passed proposal round 8, but routine does not mean stagnation. Even though the neutron guide hall west is now crowded with instruments, new projects and ideas still appear nearly every month. The planning of the instrumentation in new guide hall east is almost settled. Nevertheless, the major work for the connection of the east-building to the reactor in order to transfer neutrons and positrons remains to be done. Large projects like the ultra cold neutron source or new infrastructure buildings are emerging. A major step next year will be the increased participation of the Helmholtz centres at the FRM II leading to substantial changes in our institute.

News are exiting, but without an appropriate communication they tend to be lost in the daily business. This news letter will try to keep you informed about our latest developments concerning the usage of the neutrons in Garching. Furthermore we want to report on groups doing service and science at the FRM II. The different authors of the contributions presented here may remind you that the FRM II is based on the strong collaboration of scientific groups from all over Germany present here on-site.

Jürgen Neuhaus
Deputy Director FRM II

December 2008

Deadlines Proposal Rounds

FRM II (Nº 9)
January 16th, 2009
user.frm2.tum.de

JCNS (Nº 5)
April 6th, 2009
fzj.frm2.tum.de

CONTENTS

Improved Flux, Better Software at SPODI

During the first half of 2008 the performance of the high-resolution powder diffractometer SPODI has been improved both by a new monochromator focusing unit and a new algorithm for the data evaluation.

The new monochromator focusing unit allows continuous change of the focusing distance from 1.4 m to ∞. With this device both the flux and the profile of the incident neutron beam were improved resulting in higher counting rates of about 50 %.

With respect to data evaluation, a new algorithm has been implemented in the data treatment software to overcome asymmetric broadening effects at low scattering angles, when using the full detector height of 300 mm.

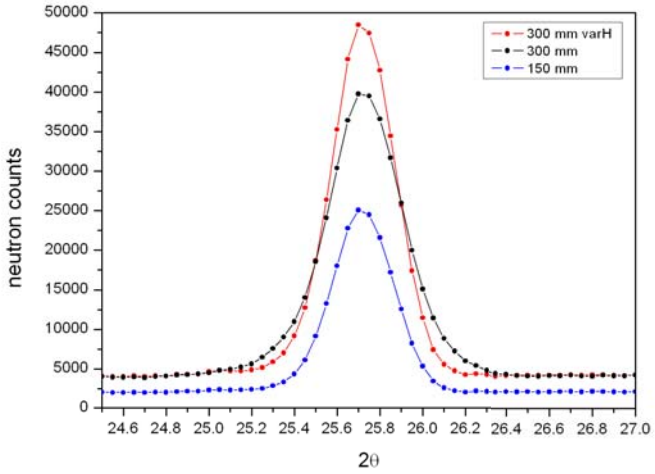


Fig. 3: Comparison of integrated peak profiles for various data extraction procedures.

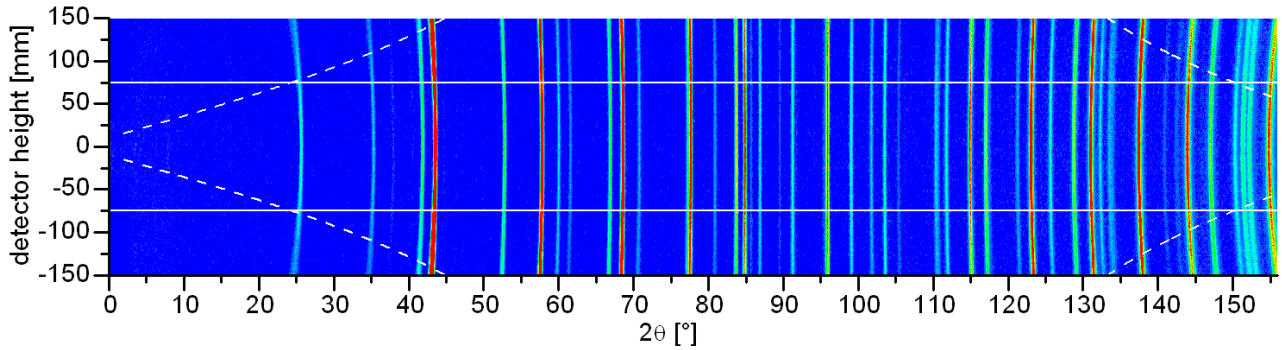


Fig. 1: Two-dimensional data set of a corundum reference sample. The straight white lines define a detector height of 150 mm and 0 denotes the centre of the detector. The dotted white lines encompass the data used in the “300 mm - variable height” data set.

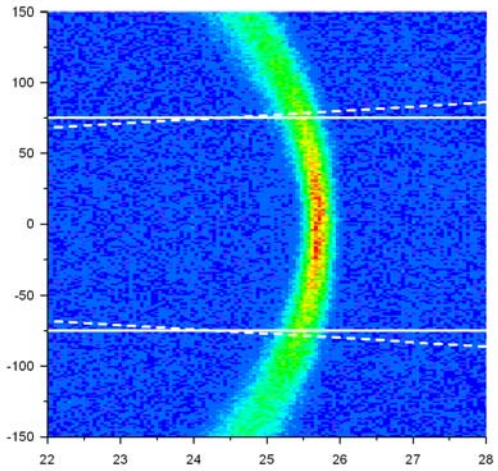
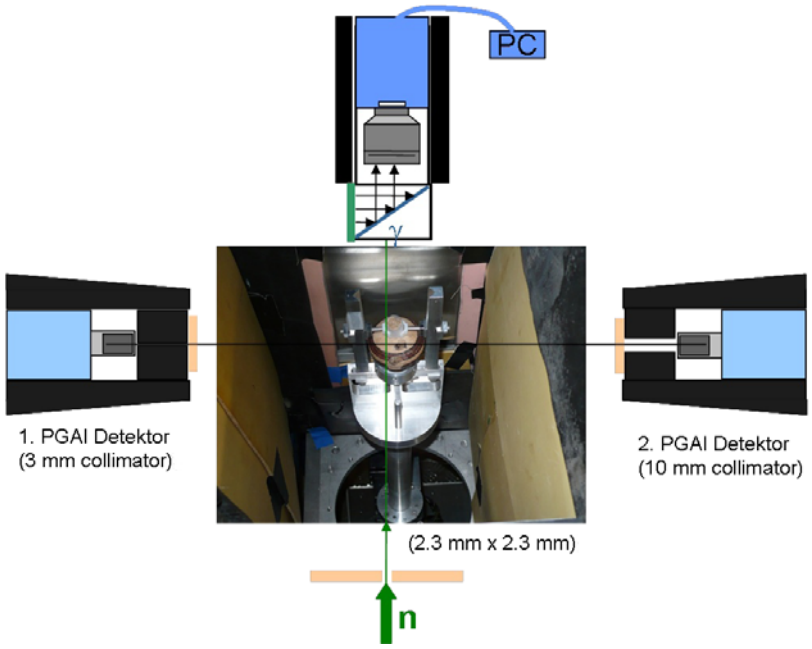


Fig. 2: The (012) reflection of corundum, enlarged section of figure 1.

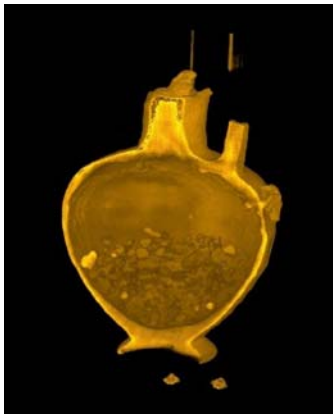
As a consequence of the vertically divergent beam and the sample height, the Debye-Scherrer rings (figure 1) are smeared out along the vertical direction, resulting in peak broadening and asymmetry especially at low and high scattering angles (figure 2). So far, good peak profiles could only be obtained by limiting the detector height to about 150 mm (the straight lines in figure 1). In order to include the full height at the less affected intermediate 2θ-range, an algorithm has been developed that uses a variable height as indicated by the dotted line in figure 1. The line used depends on the sample height and the required resolution. As seen in figure 3, improved peak profiles and higher intensities are obtained by this “variable height data” normalized to the full detector height.

Markus Hölzel, Anatoliy Senyshyn
TU Darmstadt

Unique Inspection in 3D: PGAA Facility



Schematic view of the PGAA facility with Gamma detectors on the left and right and CCD-camera for tomography in beam direction.



Tomography of a Proto Corinthian ceramic vase, 600-500 bC, found in Cerveteri, Italy.

Prompt Gamma Neutron Activation Analysis (PGAA) is a non-destructive radioanalytical technique for the determination of elemental composition of different samples. The main advantages of this technique are the shorter irradiaiton times compared to the standard Neutron Activation Analysis (NAA) and the easy preparation of the samples.

The facility uses the cold neutron beam of NL4b which has a very high intensity due to the elliptically tapered design of the beam guide. The neutrons are focused at the sample position with a maximum thermal equivalent flux of $6.3 \cdot 10^{10}$ n/cm² s ($1.7 \cdot 10^{10}$ n/cm² s using the measured mean energy of the neutron spectrum). Furthermore, two different measuring positions are available, as the last 1.1 m of the beam guide is removable. The two measuring positions have different properties: With a useable area of 14 mm x 38 mm (width x height) at a distance of 35 cm or with 4 mm x 10 mm at 9 cm.

The detection system consists of two HPGe detectors, both with a standard Compton suppression system. A low measuring background and a careful calibration of the efficiency curve ensures a good quality of analysis.

Recently, in the frame of the EU project *Ancient Charm*, a new setup was added. This new configuration allows a new type of analysis, the so called Prompt Gamma Activation Imaging (PGAI).

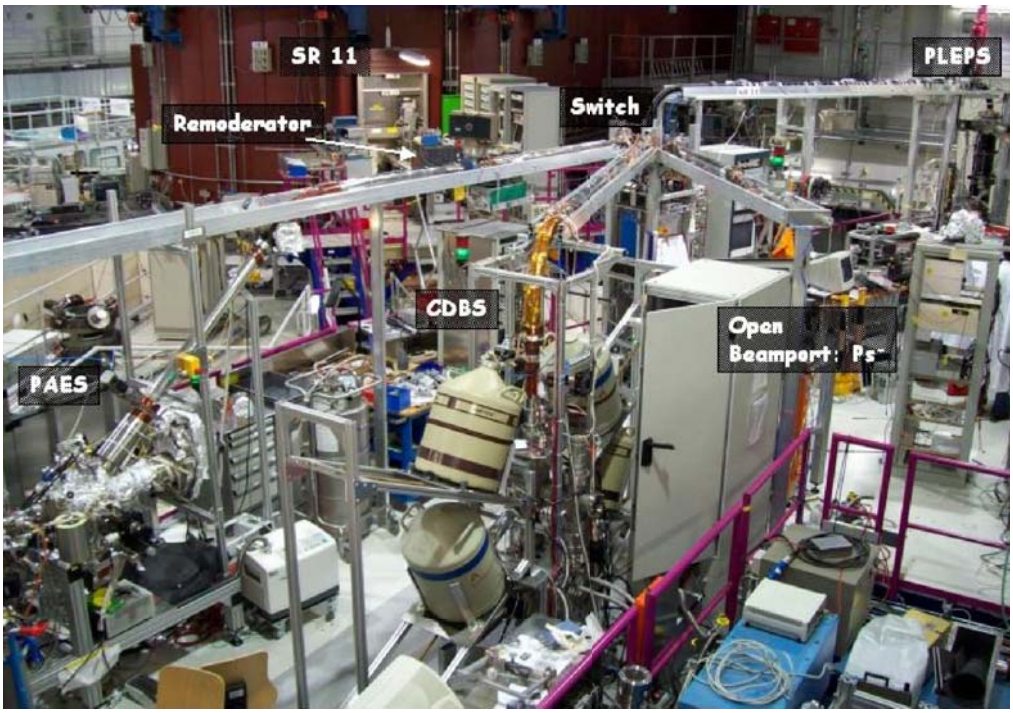
With this particular set-up position sensitive PGAA measurements reveal the spatial distribution of elements inside the object. This goal is achieved by introducing a neutron collimator that reduces the area of neutrons to a 2 mm wide spot and a gamma collimator of 3 mm in diameter in front of the HPGe detector. The intersection of these two collimators defines the active measurement volume inside the sample.

In addition to standard PGAA and PGAI, a neutron radiography system was installed. This system allows one to acquire a tomographic image of the sample and confirms also the correct positioning of the sample inside the beam through neutron radiography. The combination of tomographic imaging and 3D elemental analysis presents the new method for the analysis of historic objects.

A future development for the standard PGAA instrument is the full automation of the measuring process and the data acquisition system. Efforts will be made to further decrease the peak-to-noise ratio and the background count rate. Concerning PGAI and the Ancient Charm project, the efficiency of the system will be increased in order to be able to acquire more complete PGAI measurements on real objects coming from different museums. Another aim is to increase the spatial resolution of the PGAI system.

Petra Kudějová
Universität zu Köln

Multi-Purpose Positrons at NEPOMUC



Creative chaos on using positrons at different experimental stations.

At the start of 2008, a new in-pile gamma-converter and Pt-moderator was installed at the neutron induced positron source NEPOMUC of the FRM II. The unprecedented intensity of the moderated positron beam amounts to $(9.0 \pm 0.8) \cdot 10^8$ moderated positrons per second at an energy of 1 keV. Hence, the beam facility NEPOMUC provides the world highest intensity of a monoenergetic positron beam reported so far. Up to now, no degradation of the positron yield has been observed after several months of operation. Thus, the long-term stability of the positron beam enables a wide variety of experiments in solid state and surface physics, materials science and atomic physics with high reliability.

Presently, four spectrometers are in operation at the NEPOMUC positron beamline, and a fifth experiment is currently being installed:

Crystal defects in metals, semiconductors or insulating materials and the free volume of polymers are studied with the pulsed low-energy positron system for positron lifetime measurements (PLEPS). This unique spectrometer allows depth dependent measurements up to a few µm.

The coincident Doppler-broadening (CDB) spectrometer allows the investigation of defects near the surface and in the bulk up to a few µm with a lateral resolution between 300 µm and 2 mm. Moreover, elemental information in the surrounding of defects is gained which plays a major role e.g. for the understanding of precipitation growth in metallic alloys.

An apparatus for positron annihilation induced Auger-electron spectroscopy (PAES) was set into operation with a new electron analyser. By this challenging new technique the topmost atomic layer of surfaces can be analysed with improved sensitivity.

A multi-purpose beamport allows various experimental set-ups to be connected to the positron beamline. At present, an apparatus for the production of the negatively charged positronium ion Ps^- is in operation in order to study this fundamental bound state of three leptons.

An experimental interface is currently installed in order to enable the operation of a positron microscope, developed at the Universität der Bundeswehr München for positron lifetime studies with an enhanced lateral resolution of about 1 µm.

Christoph Hugenschmidt
FRM II

A New Beast in the Guide Hall: J-NSE

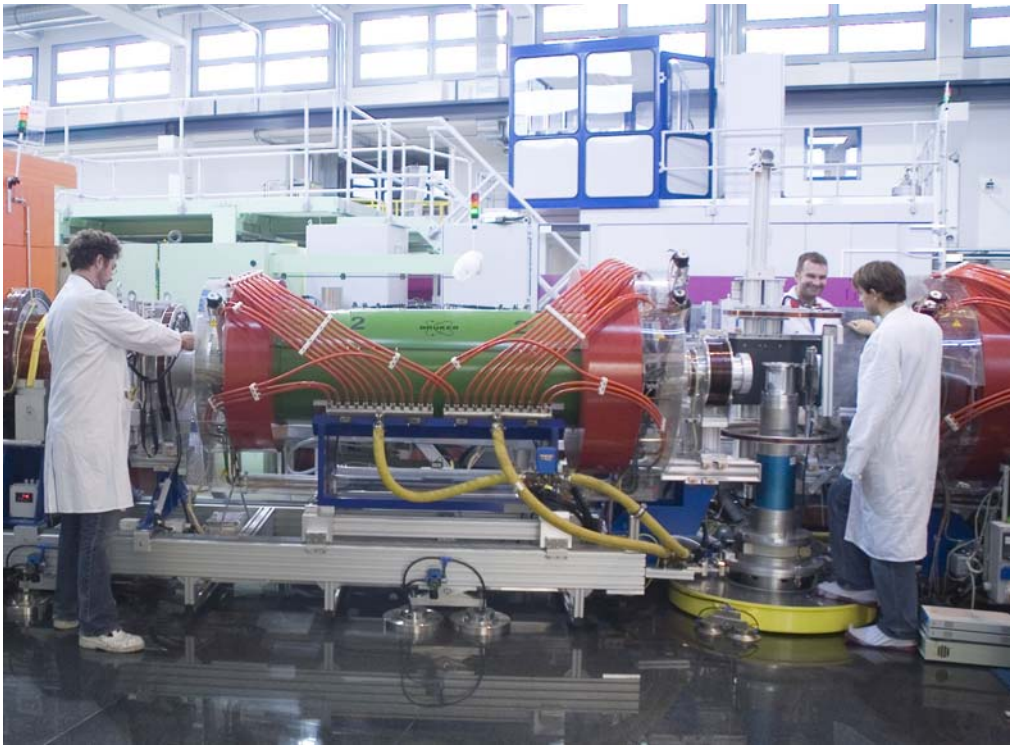


Fig. 1:
Sample stage and second arm of the J-NSE spectrometer with the main precession coil (green).

The neutron spin-echo spectrometer J-NSE provides very high energy resolution and is therefore well suited for slow processes of mesoscopic objects. Spin manipulations of the neutrons are used to convert tiny velocity changes of the neutron during the scattering process into changes of the polarization of the neutron beam. Figure 1 shows the main precession coil of the second arm of the spectrometer.

Since its restart after the relocation from the Jülich reactor FRJ-2 to the FRM II at Garching, experiments have been carried out in different fields of soft matter physics such as polymer dynamics, confinement effects, microemulsions, micelles and microgels, and also first experiments of the dynamics of paramagnetic samples have been conducted. Figure 2 shows an example of the dynamics of the surfactant layer in a bicontinuous, sponge like microemulsion which allows the determination of the bending rigidity of the membrane.

The new end position in the neutron guide hall of the FRM II provides a very intense neutron beam with a 15 fold gain of intensity at the sample position compared to the setup in Jülich at the same wavelength.

The accessible q range is 0.02 to 1.7 $Å^{-1}$, corresponding to distances of interest from 0.37 to 30 nm. Fourier times between 3 ps and 150 ns can be accessed at the moment due to the possibility of varying the wavelength at the end position of the neutron guide. Ongoing development will improve correction coils which will allow the use of higher field integrals and therefore increasing the dynamic range of the spectrometer.

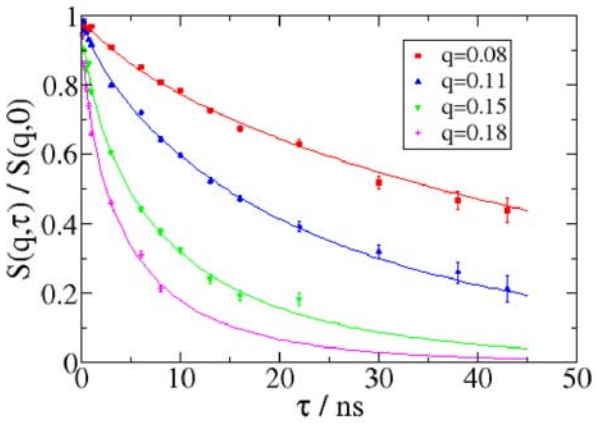


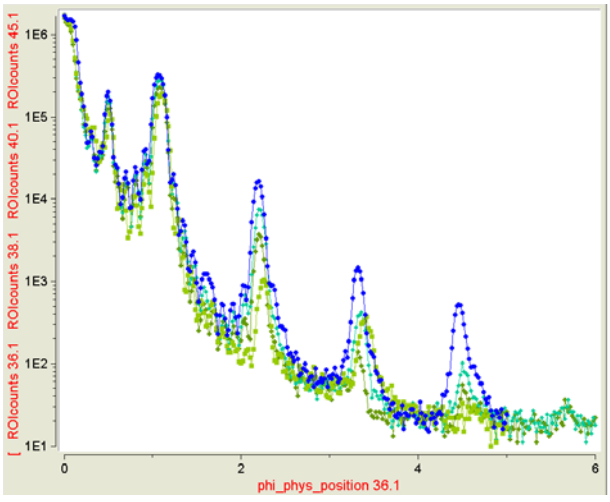
Fig. 2: Intermediate scattering function of a bicontinuous microemulsion measured at a wavelength of 8 Å

Olaf Holderer
JCNS, Garching

Combining Neutrons and X-rays in Reflectometry: N-REX+

The Great Escape of Neutronosaurus Rex from the box, frightened by polarized neutrons.

The combined neutron and X-ray reflectometer N-REX+ of the Max-Planck-Institut für Metallforschung has become operational. The project is part of the joint initiative of several Max Planck institutes at the FRM II for a focused research programme exploiting the unique properties of neutrons for the investigation of advanced materials and condensed matter phenomena.



Neutron reflectivity results obtained on a nickel / titanium multilayer after different heat treatments.

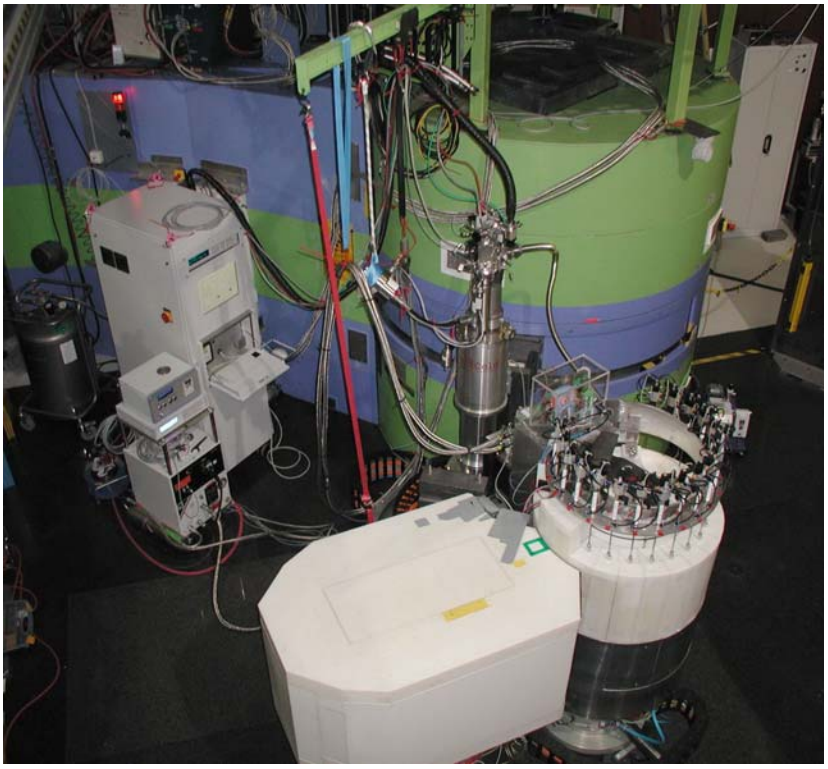
The instrument is located in the neutron guide hall at the cold guide NL1. It is equipped with a focussing HOPG monochromator using wavelengths in the range 2 Å to 6 Å.

Its design enables experiments with polarized neutrons, including wide angle neutron spin analysis and specular and off-specular reflectivity measurements on surfaces and interfaces of solid and liquid samples. In addition grazing incidence and evanescent wave diffraction measurements can be taken. As an option, in-situ X-ray characterization and spin-echo resolved grazing incidence neutron scattering (SERGIS) are available.

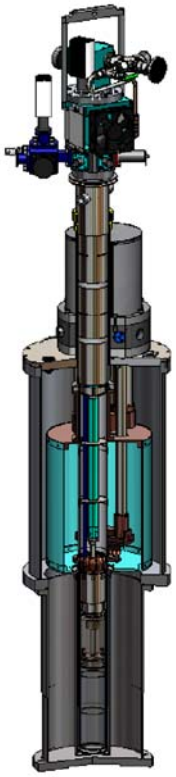
For horizontal and vertical sample orentation standardised environments including high magnetic fields up to 7.5 T, medium temperatures with liquid thermostat for cooling and heating and low temperatures down to at least 4 K can be used. Low pressure gas atmospheres at T < 300 °C and a medium pressure (p < 10 bar) gas cell with silicon substrate are routinely provided. For special experiments a large diameter (100 mm) silicon liquid film cell (T < 100 °C) and an active anti-vibration device for experiments on free liquid surfaces can be used.

Adrian Rühm
MPI für Metallforschung, Stuttgart

Sub-Kelvin Temperature Routinely Available



The ^{3}He-insert in operation at the instrument PANDA. No limitation of the insert is given concerning the tilt of the cryostat as frequently used at the three-axis spectrometers. In addition to the He compressor (left) the gas handling system (rack of 60 cm by 80 cm and 220 cm height) with pumps and compressors for the ^{3}He can be seen behind.



For scientific experiments at the FRM II changing temperature is the most requested and in terms of milli Kelvin measurements one of the most demanding parameter. The sample environment group in collaboration with an external company have developed cryo-liquid free cryostats that are now in operation at nearly all instruments. These top loading cryostats achieve a lowest temperature of about 3 K solely by pushing a single button. This ease of operation has been the paradigm of the new ^{3}He sample stick insert which extends the lowest temperature down to around 400 mK.

The low temperatures, however, need special care for mounting the assembly prior to the experiment which takes normally half a day. For measuring times of about one day using the single shot mode of the ^{3}He filling, lowest temperatures down to 380 mK have been achieved while in continuous operation 450 mK over several weeks are possible.

The strong cooling power of 1 mW, even at 500 mK, permits one to cool down most of the samples investigated from 3 K down to the lowest temperature within 10 min. This has been advantageous during a recent experiment at the single crystal diffractometer RESI where frequent temperature changes from 0.5 K to 8 K were requested.

“A stable and reliable operation for the low temperature inserts has been our main ambition for this development”, says Jürgen Peters, head of the sample environment group.

All together two ^{3}He low temperature inserts are available for routine operation, one further is under construction. The design of the cooling stage allows easy modification in order to meet special requirements for user experiments like gas adsorption on the sample or in-situ pressure variation.

Full remote control of the ^{3}He-system is allowed by the gas handling equipment. This concerns not only the integration of the temperature control into the instrument software but as well remote trouble shooting for the members of the sample environment group if requested out of working hours.

Jürgen Neuhaus
FRM II

8th German Neutron Scattering Conference

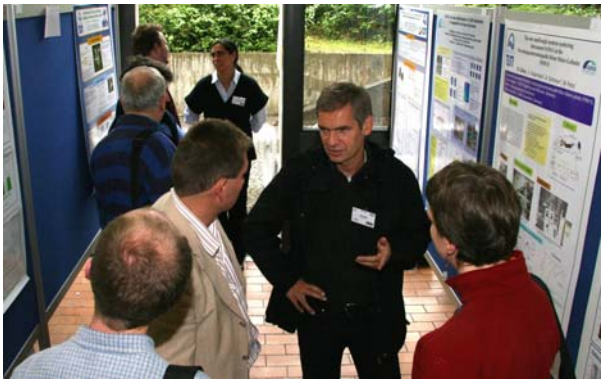
September 15-17, 2008 - Garching

The 8th German Neutron Scattering Conference was held on the 14-17 September 2008, organised by FRM II at Garching near Munich. It was a joint event of the German and Austrian Committees for Research with Neutrons, gathering 261 participants. Plenary talks and two parallel sessions dealing with the broad range of topics inherent to neutron scattering made up the programme, including 2 poster sessions on Monday and Tuesday, presenting 251 contributions. Special mini-symposia had been organised to highlight current topics in solid-state physics: "Function from Frustration in Modern Multiferroics", "Dynamics, Kinetics, Complex Materials in the Light of SANS and Reflectometry" and "Materials Science" with the focus on applied science.

Obviously, the event's interest focused strongly on the development of new methods and instruments using neutrons. A special session was dedicated to the new spallation sources SNS, ISIS's second target station and the developments related to the eagerly anticipated European Spallation Source. Topical sessions covered magnetism, soft matter, materials and dynamics.

All participants enjoyed the dinner in the *Hofbräukeller* and Richard Wagner, director of the ILL, provided a memorable speech about the world of soccer quoting sentences from prominent players.

At the conference dinner, Götz Eckold, Universität Göttingen, the new head of the Committee for Research with Neutrons, thanked Helmut Schober, ILL, for his excellent work and engagement during the past three years.



Ralf Gilles, FRM II explaining the use of the future small angle scattering machine SANS-1 to potential users.

Wolfram-Prandl-Prize 2008

Presentation of the Wolfram-Prandl prize to Michael Marek Koza (second from left) by the head of the German Committee for Neutron Research Helmut Schober (right) in the presence of Winfried Petry (scientific director of the FRM II) and Ina Lommatzsch (FRM II User Office).

Since 2002 the Wolfram-Prandl prize has been awarded to young scientists who have done outstanding work in the fields of neutron scattering, method development or fundamental physics with neutrons. Presented at the bi-annual German neutron scattering conference, the prize money of 2,500 Euro is equally funded by the neutron centres GKSS, HMI, FRM II, JCNS and ILL. The 2008 Wolfram-Prandl prize was awarded to Michael Marek Koza of the ILL for his outstanding work on the structure and dynamics of crystalline and amorphous ice. In his prize lecture he gave an overview of the temperature-pressure phase diagram of the still fascinating substance water and shed more light on the miracle of high- and low-density amorphous phases of ice.

Jürgen Neuhaus
FRM II

Open Day 2008

October 18, 2008 - Research Campus Garching

Queuing up for two hours, handing in their passports and coming back at a certain time - hundreds of people gladly did so at the open doors of the neutron source FRM II. From 10:00 to 19:00 on Saturday, 18th October, in total 488 visitors had a look inside the reactor, the experimental and the neutron guide hall.

In 32 groups of 15 people and in 15-minute cycles they got to know more about the research at the neutron source. The interest in visiting the reactor was so huge, that three hours after the start of registration on the visitor groups were fully booked. When the lists were full, some visitors even waited for hours, just in case somebody would not show up, to get a chance to visit the reactor.

Long lines for the registration at FRM II. By noon, all tours at the neutron source were fully booked.

A lot of attention was attracted by the presentations of the FRM II-radiation protection group. Three staff members constantly explained the safety concept of the neutron source and how measurement of radiation takes place.

Public talks given by the scientific director, Winfried Petry, the deputy director, Jürgen Neuhaus, and the former technical director, Klaus Schreckenbach, were well received. The audience came to know the newest scientific highlights of FRM II, the use of positrons in materials science and atomic physics and general aspects of the application of neutrons.

Andrea Voit
FRM II

Workshop

Biomolecular Dynamics and Protein-Water Interactions

September 24-26, 2008 - Feldafing

More than 60 scientists from Europe, USA, Australia and Japan attended the international workshop on *Biomolecular Dynamics and Protein-Water Interactions* on September 24-26, 2008 in the beautiful surrounding of the InWent Education Center close to Lake Starnberg south of Munich.

The workshop was jointly organized by Wolfgang Doster of Physics Department of Technische Universität München, and Thomas Gutberlet of Jülich Centre for Neutron Science. Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) and Forschungszentrum Jülich GmbH gave generous financial support.

The focus of the workshop was the discussion of the mechanism of the protein dynamical transition, protein hydration and protein dynamics studied by neutron scattering and other methods.

The highlights of the workshop were intense discussion between the participants, an evening poster session and a visit of the Roseninsel in Lake Starnberg after the end of the workshop.

Most participants appreciated the open and informal way to discuss current competing dynamic models and experimental approaches to study protein dynamics.

A clear demand for more sophisticated neutron experiments to study dynamical phenomena in proteins and biological systems was expressed. Regarding the use of neutron spectroscopy in the field of water dynamics the participants were very delighted with recent developments to use of new instruments such as the time-of-flight spectrometer TOFTOF or the backscattering instrument SPHERES. Combining these techniques with dedicated simulation efforts and complementary NMR studies to gain more insight into protein and water dynamics is clearly going to be a strong topic for the future.

Thomas Gutberlet
JCNS, Garching

DGK (AK7) Workshop
Neutrons for Crystallographers
September 17-18, 2008 - Garching

The well attended lecture hall at the Physics Department of Technische Universität München at Garching

The working group *Neutron Scattering* (AK7) of the German Society for Crystallography (Deutsche Gesellschaft für Kristallographie, DGK) held the workshop *Neutrons for Crystallographers* following the 8th German Neutron Scattering Conference at Garching at Technische Universität München from 17th to 18th September 2008.

The workshop was aimed at students and scientists of the different disciplines in natural and materials sciences. A general introduction to the use of neutrons was given, followed by the application of neutrons for the research in different scientific topics.

On the first day the analysis of atomic and magnetic structures using neutron diffraction was explained. During four lectures, two on powder methods and two on single crystal diffraction, subdivided into structure determination and magnetism (R. Gilles, A. Schneidewind, M. Meven, M. Braden). On the second day four lectures were held on phonons and magnons, diffuse scattering, material science and soft matter (M. Braden, F. Frey, W. Brokmeier, V. Haramus).

Details were given about the instruments for the different applications during a guided tour of the neutron source Heinz Maier-Leibnitz (FRM II) after the lectures.

The workshop was very well attended. Beside the numerous participants from all over Germany and beyond (Aachen, Augsburg, Braunschweig, Dresden, Freiberg, Köln, München, Regensburg, Göttingen, Innsbruck) attendees of the neutron scattering conference joined the workshop. Thus, more than 50 participants filled the lecture hall. There were many questions after the lectures and lively discussions between the audience and the speakers in the breaks between the lectures. This underlines the large interest in the methods presented as well as the successful mixture of lectures, discussions and guided tour of a research facility.

With the support of FRM II and DGK this workshop could be realised without any participation fee.

Martin Meven
FRM II

JCNS Workshop 2008
Modern Trends in Neutron Instrumentation
October 15-17, 2008 - Bernried

New developments and concepts in neutron scattering instrumentation was the topic of a well received recent workshop organized by the Jülich Centre for Neutron Science. More than 60 scientists from neutron facilities across the world joined the event in the conference hotel Seeblick at Bernried at Lake Starnberg.

The workshop covered concepts and challenges in neutron instrumentation for spallation neutron sources as well as reactor sources. New projects and developments in small angle neutron scattering, neutron diffraction, neutron spin echo spectroscopy, backscattering and time-of-flight spectroscopy, neutron reflectometry, neutron polarization and Larmor techniques and simulation techniques were presented. Lively discussions accompanied the presentations and intense poster session.

Lively discussions at the poster session at Bernried

Several instruments and projects at the FRM II were presented within the workshop: the diffuse polarised spectrometer DNS (JCNS), the polarized diffractometer HEIDI (RWTH Aachen), the POWTEX diffractometer project (RWTH Aachen, Universität Göttingen), the TRISP spectrometer (MPG), MIRA (TUM), the relaunched Jülich NSE instrument, KWS-2 SANS instruments of JCNS, TOFTOF (TUM), the future thermal time-of-flight spectrometer TOPAS (JCNS), the new backscattering instrument SPHERES (JCNS), the new reflectometer MARIA (JCNS) and the reflectometer N-REX$^+$ (MPG).

On the second day the workshop visited the FRM II facility at Garching where the participants joined the local instrument responsibles for intense discussions on site. Afterwards the participants relaxed at the workshop dinner where an introduction to the history of Bavarian beer brewing was given.

The workshop participants agreed to collect the presentations given during the workshop and to make them available at the workshop webside

www.jcns.info/Workshop

to allow the general neutron community to follow the discussions.

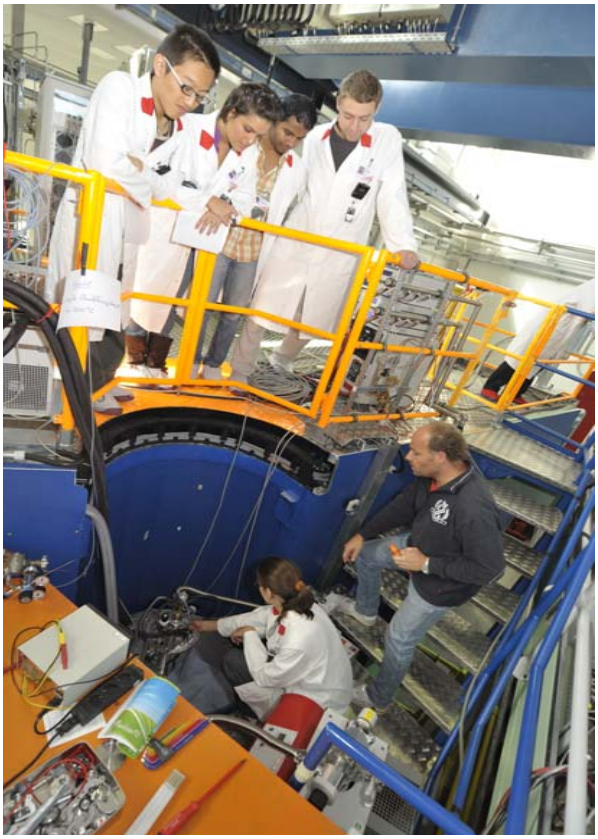
Thomas Gutberlet
JCNS, Garching

12th JCNS Laboratory Course Neutron Scattering

September 1-12, 2008

The 12th Laboratory Course on Neutron Scattering was held by the Jülich Centre for Neutron Science September 1–12. The lectures took place at Forschungszentrum Jülich and the experiments were carried out at the FRM II. 50 young students and scientists from a variety of disciplines such as physics, chemistry etc. from all around the world took the chance to learn theory and hands-on neutron scattering on selected instruemnts at FRM II. The course was supported by the Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3) and SoftComp, the European Network of Excellence for Soft Matter Composites.

The lectures gave a comprehensive introduction to neutron sources, into scattering theory and instrumentation. Furthermore, selected topics of condensed matter research were presented. At FRM II the students performed experiments at the backscattering instrument SPHERES, the neutron reflectometer TREFF, the Jülich neutron spin-echo spectrometer J-NSE, small angle scattering at KWS-2, single crystal and powder diffraction at HEIDI and SPODI, polarisation analysis at DNS, zero field spin echo spectroscopy at RESEDA, three-axis spectroscopy at PUMA and time-of-flight spectroscopy at TOFTOF.



Interested students keeping an eye on TOFTOF's sample environment (above), enjoying data treatment at DNS (left) and looking SPHERES over (bottom).

The response was overwhelmingly positive. The splitting of the locations was surprisingly not seen as a burden although it implied a daylong bus trip from Jülich to Munich. Rather the students appreciated the possibility to get to know two major research centres in Germany.

The next Laboratory Course will be held again at Jülich and Garching on September 7-18, 2009.

Thomas Gutberlet
JCNS, Garching

FEMaS: Neutrons and Positrons for Fusion Energy

October 8, 2008 - Garching

Lively discussions already during the registration of the kick-off meeting in Garching.

In a Coordination Action, the Euratom seventh framework programme for nuclear research and training has launched the FEMaS-CA on October 1, 2008. The development of fusion energy is strongly correlated to the development of new materials for the fusion chamber of the reactor. The main concerns are structural materials to resist the neutron irradiation and maintain mechanical stability up to high temperatures in addition to a low activation property. In addition plasma-facing materials have to be engineered in order to remove the high heat fluxes. Coatings have to be developed for electrical insulation and corrosion resistance under irradiation and in contact to liquid cooling metals.

The FEMaS coordination action wants to improve the use of advanced materials characterisation methods such as neutron and synchrotron radiation as well as high resolution TEM and the use of positrons for defect characterisation. The consortium as a whole is divided into 5 work packages dealing with radiation damage, synchrotron based methods, neutron source based methods including positrons, TEM based methods and advanced mechanical testing and characterisation.

A first kick-off meeting was held on the 8th October 2008 at the Max-Planck-Institut for Plasma Physics at Garching. Besides plenary sessions dealing with general aspects concerning the organisation and presentations from EU officers, the work package groups met for a first exchange of envisaged projects from the fusion energy community and large scale facilities offering the advanced characterisation methods.

The neutrons and positrons offered by FRM II are coordinated by Christoph Morkel

contact: **christoph.morkel@frm2.tum.de**

A first workshop to present and discuss upcoming developments and possible collaborations will take place in Lisbon on January 12-14th, 2009.

Jürgen Neuhaus
FRM II

From Molecular Motions to Pharmaceutical Products: TOFTOF in motion

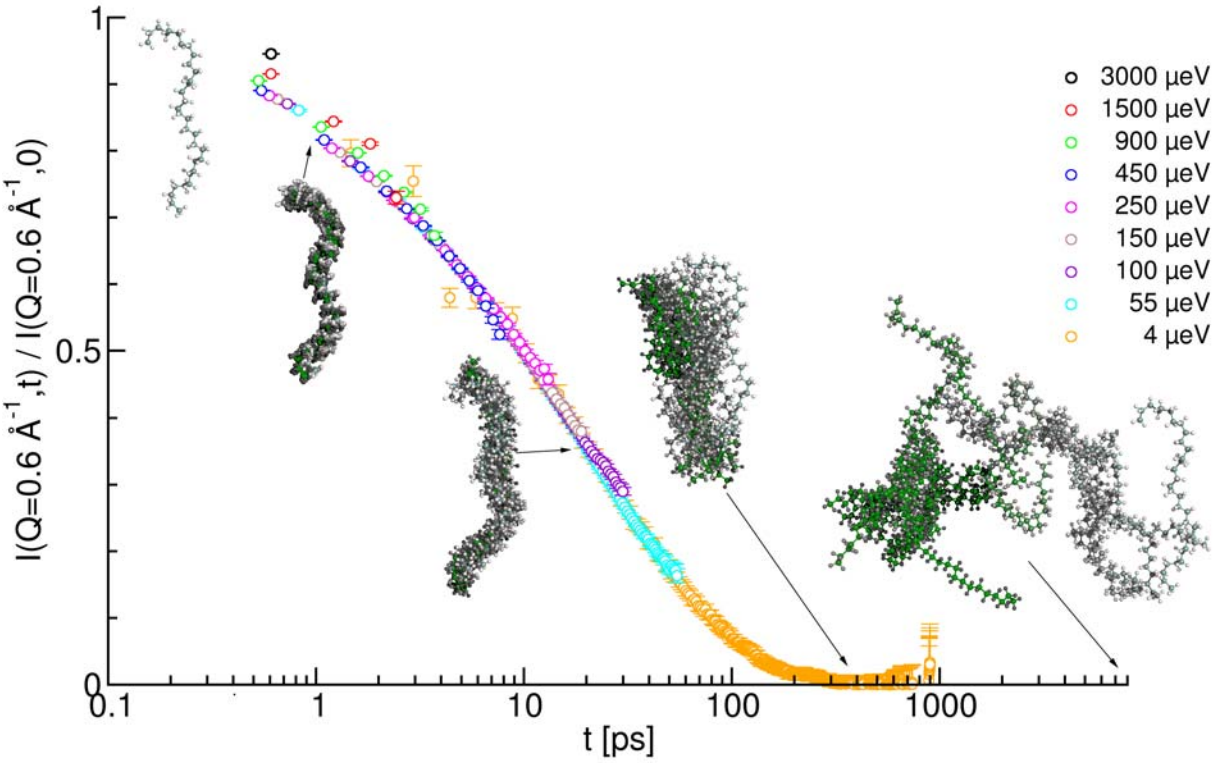
The TOFTOF team in front of the instrument.

With the beginning of routine operation of the TOFTOF spectrometer in 2005 the first efforts have been made to establish a small research group at the spectrometer. The research is focussed on studies of molecular motions and the spatial arrangement of organic molecules in dispersions used in pharmacy as carrier systems for drug delivery but also in the food industry and other applications.

The first studies included experiments on the dynamics of liquid (bulk and dispersed) phases of simple molecules like oils and fats but also on the motions of stabilizer molecules or other additives such as drug molecules in pharmaceutical formulations. From these studies a better insight to the transport mechanism of the molecules in simple molecular liquids but also in phospholipid mono- and bilayers could be achieved. The understanding of the microscopic structure and dynamics should help to optimize macroscopic physico-chemical properties of, e.g., pharmaceutical products such as drug release rate or dispersion stability.

Due to the fact that dispersions are metastable systems it is essential to have the possibility to prepare and characterize the samples on-site. For that purpose besides the basic laboratory equipment provided by FRM II some special apparatuses were granted by the “Bund der Freunde der Technischen Universität München eV” which also financed the first Ph.D. student in that project over a one year period.

Using a neutron time-of-flight spectrometer for studies on the molecular dynamics of native pharmaceutical systems for intravenous administration was a novel idea. It had to be demonstrated first that quasi-elastic neutron spectroscopy (QENS) is well suited to reveal properties of systems relevant for pharmaceutical science. Already with the first quasi-elastic time-of-flight neutron scattering (TOF-QENS) experiments it could be demonstrated for a co-enzyme Q_{10} nano-emulsion stabilized by phospholipids in an aqueous phase that it is possible to measure in detail the molecular motions inside the nano-sized droplets of dispersions. It turned out that the observed results are not only relevant for the pharmaceutical applications but also of general interest from physical point of view. Therefore, a systematic study on the picosecond dynamics as probed by TOF-QENS of medium-chain n-alkanes was initiated.



Intermediate scattering function of the n-alkane $C_{32}H_{66}$ at 90°C measured with the TOFTOF spectrometer using the labeled instrumental resolutions (FWHM of the elastic line). Representative trajectories of a single molecule as extracted from MD simulations of the same liquid alkane are plotted for time ranges between 0 ps and 1 ps, 20 ps, 400 ps and 8 ns, respectively. The time evolution is indicated for each picture by colour intensification. For each picture 20 snapshots of the molecule equidistant in time are overlayed.

Including additional molecular dynamics (MD) simulations different diffusive motions could be disentangled in such liquids ranging from fast tumbling of CH_2 to the long range molecular diffusion. Despite the rod like shape of the molecules the centre-of-mass diffusion was found to be essentially isotropic.

TOF-QENS studies are also helpful for the understanding of the molecular transport properties in biological membranes and stabilizer layers in dispersions. Evidence was found that the long range motion on a picosecond time scale has a flow-like character. This result confirms recent MD simulations experimentally and adds another piece of knowledge to the understanding of lateral diffusion of molecules in membranes.

The interpretation of the dynamics of phospholipid molecules in the stabilizing layer of emulsions is, however, difficult without the knowledge of the structural arrangement of the molecules. For this purpose a special evaluation method of small angle X-ray scattering (SAXS) experiments (X-ray powder pattern simulation analysis, XPPSA) has been developed and first results of phospholipid layers surrounding solid triglyceride nano-particles have been achieved. The continuation of this project is now supported by the DFG for three years and a collaboration with the Department of Pharmaceutical Technology of the Technische Universität Braunschweig has been established in order to correlate our results with pharmaceutical parameters of relevant systems.

Today, the small TOFTOF research group consists of two PhD students, one diploma student, the group leader and several working students. It has strengthened the in-house research at the TOFTOF spectrometer and already within the first three years a lot of valuable insights in the molecular dynamics of colloidal dispersions have been gained. A list of recent publications can be found under

www.e13.physik.tu-muenchen.de/unruh

Tobias Unruh
FRM II

The Radiation Protection Team

New head and new structure

FRM II's radiation protection team. Rightmost: The new head Birgit Wierczinski

Access to the neutron source for users has and will become smoother with the new regulations in radiation protection. This is one of Birgit Wierczinski's aims. Recently the radio chemist became the new head of reactor supervision and radiation protection officer. Her predecessor Helmut Zeising retired.

Birgit Wierczinski was born in Freiburg im Breisgau. She studied chemistry at her home town's university and at ETH Zürich. After her Ph.D. in Mainz in 1994 Birgit Wierczinski accepted post-doc positions in the USA, Sweden and became a staff member at TU Delft in the Netherlands. Since 2003 she worked at the Institute for Radiochemistry at Technische Universität München and became staff member of FRM II in 2007.

The radiation protection division at FRM II was restructured. The staff members now are divided into four subdivisions:

- applied radiation protection,
- in-house chemistry,
- radiation protection services and
- dosimetry of persons.

Scientists usually get involved with radiation protection for either personal dosimetry or contamination control. Personal dosimetry at the FRM II is done using a combination of daily read-out electronic dosimeters and the monthly analysis of film badges. Contamination control includes regular testing of instruments inside the experimental areas as well as clearance measurements of all equipment leaving these areas. Samples that have been in the neutron beam are more carefully analysed by gamma-spectrometric methods.

Of course, the function of reactor supervision is not only radiation protection. The 23 staff members exercise many duties. For instance, waste water, which is produced within the control area of the FRM II is chemically monitored by the in-house chemistry. Radiation protection services organizes the disposal of radioactive waste and cleans sensitive areas. Two members of the team take care of the laundry of overshoes and lab coats. The applied radiation protection team monitors the environment of the neutron source. Probes of water, soil and plants are taken to control the intake of radioactivity in the surrounding of FRM II. Also, radiation protection ensures, that no radioactive particles are incorporated by users or staff in FRM II. Radiation at workplaces is surveyed daily by measuring of the dose rates as well as wipe testing for contamination control. Regularly, all measuring instruments, such as whole body and contamination monitors, dose rate meters, spectrometers, analytical equipment etc., have to be tested and calibrated for correct operation.

Andrea Voit
FRM II

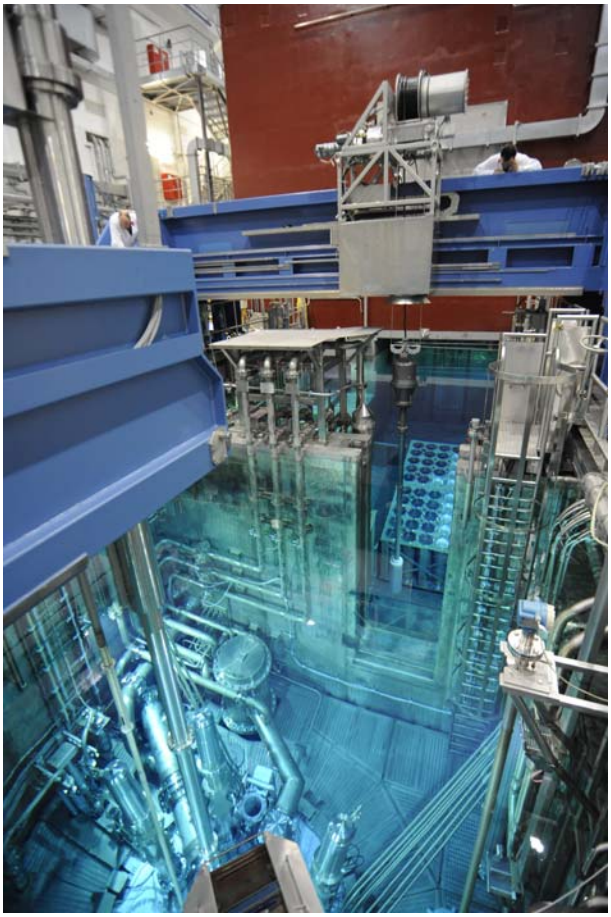
Improved Silicon Doping Facility

More security and higher output with semiautomatic system

Recently the doping of silicon at FRM II uses a new semiautomatic system. It replaces a mechanical device for charging the irradiation position with Si-ingots.

The new system moves the single crystalline Si ingots between the irradiation channel located in a thimble within the D_2O moderator tank and the storage rack within the pool following predefined tracks. “The handling of the silicon crystals has become easier than before”, says Heiko Gerstenberg, head of the irradiation group at FRM II. Another advantage of the semi-automatic system, which had total costs of about one million Euros: The output of doped silicon has gone up by several tons compared to the slower mechanical system. This year, Heiko Gerstenberg hopes to reach the mark of 10 tons of doped silicon.

In two shifts six irradiation technicians overlook the production of doped silicon weekdays from 5:30 to 22:30. The products serve the semiconductor industry in Europe and Japan as raw material.



The ingots move from their irradiation position within the moderator tank to the storage rack within the reactor pool.

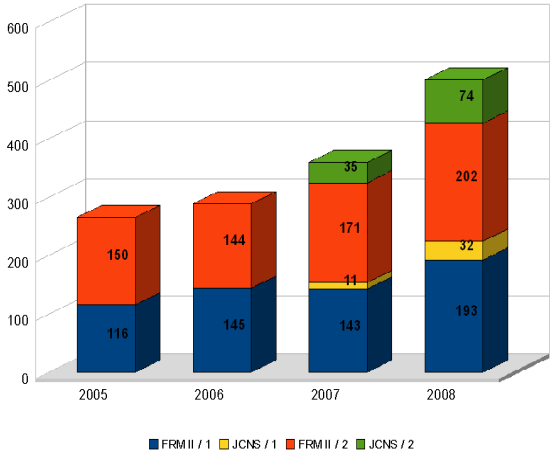
The semiautomatic system is controlled by the supervising technican.

The semiautomatic device transports the silicon ingots to defined spots in the reactor pool. An irradiation technician has to manually trigger the step by step transportation towards the storage rack or the irradiation channel. The human control ensures that a collision with unforeseen obstacles in the water, which the machine does not recognize, is avoided. The irradiation technician stands on a bridge spanning over the reactor pool to control the movements of the system.

A silicon crystal after the doping.

Andrea Voit
FRM II

User Development at FRM II



Submitted proposals 2005-2008 (FRM II and JCNS).

Since the start of the operation of FRM II in May 2005 request for beam time at FRM II instruments, the number of submitted proposals and visits of users for experiments have been increasing continuously. In 2008 external users submitted 501 proposals to FRM II and JCNS. Summing up the scientific users more than 1000 researchers will have been at FRM II in 2008. Most users are from German universities and research centres, but about 40 % of the proposals of every round are from Europe or overseas as Japan, USA or India.

To organize this amount of proposals and user visits a joint User Office of FRM II and JCNS was established in 2008. The user office handles all administrative aspects of submission and reviewing of the proposals. It provides help and information for users for their stay at FRM II and organizes travel reimbursement and NMI3 support for European users. All information for FRM II and JCNS users is regularly updated at the user office web pages:

user.frm2.tum.de
fzj.frm2.tum.de

The next User Meeting will take place on May 25, 2009 at Garching. Users are invited to present their recent results. This will be a good possibility to discuss new projects with the local contacts. Details on new opportunities and ongoing developments will be given by the large number of groups operating the instruments at FRM II:

Groups and institutions at FRM II.

Call for Proposals

January 16, 2009 is the next deadline to submit proposals for beam time at instruments at FRM II. Proposals can be submitted for the following instruments:

Diffraction:	HEIDI, RESI, SPODI, STRESS-SPEC
Reflectometry:	MIRA, N-REX$^+$, REFSANS
Spectroscopy:	TRISP, PUMA, PANDA, TOFTOF, RESEDA
Imaging:	ANTARES, NECTAR, PGAA
Positrons:	NEPOMUC
Particle physics:	MEPHISTO

Details of the instruments and sample environment available can be obtained from our website

www.frm2.tum.de

The review of the proposals will take place on March 6, 2009. Results of the referees will be online about two weeks later. The experiments of the accepted proposals will start from the 20th cycle, i.e. from June 2009 on.

The beam time on the instruments of the JCNS facility hosted at FRM II neutron source at Garching are distributed through the JCNS proposal system

fzj.frm2.tum.de

(next deadline is April 6, 2009) for the instruments KWS-2, J-NSE, DNS and SPHERES.

Thomas Gutberlet
JCNS, Garching

Reactor Cycles FRM II 2009

Cycle	Period
18b	January 5 – 29
19	March 10 – May 8
20	May 26 – July 24
21	August 18 – October 16
22a	November 17 – December 23

Upcoming

February 10-13, 2009
9th International Conference on Quasielastic Neutron Scattering QENS 2009 (Villigen/ Switzerland)
qens2009.web.psi.ch/

February 25-27, 2009
Workshop on Neutrons and X-rays meet biology (Berlin/ Germany)
www.helmholtz-berlin.de/events/biology/

March 9-20, 2009
40th IFF Spring School: Spintronics - From GMR to Quantum Information (Jülich/ Germany)
www.fz-juelich.de/iff/fs2009

March 26- Apr. 3, 2009
50th Berlin School on Neutron Scattering (Berlin/ Germany)
www.helmholtz-berlin.de/events/nschool2009/

May 3-7, 2009
International Conference on Neutron Scattering ICNS (Knoxville/ USA)
neutrons.ornl.gov/conf/icns2009/

May 25, 2009
FRM II User Meeting (Garching/ Germany)
user.frm2.tum.de

September 7-18, 2009
13th JCNS Laboratory Course - Neutron Scattering (Jülich and Garching/ Germany)
www.fz-juelich.de/iff/wns_lab_now/

Deadlines Proposal Rounds

FRM II (No 9)
January 16th, 2009
user.frm2.tum.de

JCNS (No 5)
April 6th, 2009
fzj.frm2.tum.de

IMPRINT

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Crystal ball gazing in wintertime