



# FRM II news

# N° 2



## Joined Forces

In 1997 the Technische Universität München (TUM) and the Federal Ministry of Education and Research (BMBF) launched a call for proposals to build the first 14 instruments to be operated at the FRM II. Scientists from universities and national laboratories submitted their ideas on how to use the intense neutron beams for the source under construction at that time.

Following workshops and finally the advice of the Instrumentierungsausschuss under the guidance of Prof. Dr. Tasso Springer ten instruments were selected to be realised by resources from the TUM and a further four financed by the BMBF. Subsequently the Max Planck Society agreed to support a further two instruments. Finally in 2004 FZ Jülich decided to move its best instruments from DIDO to FRM II and in the long will operate a total of nine instruments in Garching. Today 21 instruments are operational and another nine are under construction.

Designed as a national facility the State of Bavaria covered to a large extent the costs of construction and operation until now. With the increasing participation of the Helmholtz centres in Jülich and Geesthacht due to the shut down of their own sources in 2006 and 2010, respectively, the BMBF will substantially contribute to the scientific use of the FRM II. This will ensure an adequate operation and service at our instruments including future technical developments.

In future the TUM and the Helmholtz Association share in a close cooperation the scientific exploration of FRM II. Besides FZ Jülich and GKSS-FZ Geesthacht, HZ Berlin will participate as well. This cooperation will maintain the strong collaboration with University groups and Max-Planck-Institutes from all over Germany. Continuous instrument development driven by the requirements of cutting edge research will be guaranteed by this joined effort.

Winfried Petry  
Scientific Director

July 2009

## Deadlines Proposal Rounds



**FRM II (N° 10)**  
**July 17<sup>th</sup>, 2009**  
[user.frm2.tum.de](http://user.frm2.tum.de)



**JCNS (N° 6)**  
**September 14<sup>th</sup>, 2009**  
[fzj.frm2.tum.de](http://fzj.frm2.tum.de)

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## Measuring the Nanoworld

### The High Intensity - High Resolution SANS Diffractometers of JCNS at FRM II



KWS-1 and KWS-2 SANS diffractometers in the neutron guide hall of FRM II.

The small-angle neutron diffractometers KWS-1 and KWS-2 have been rebuilt by the Jülich Centre for Neutron Science (JCNS) at the FRM II. Both instruments are 42 m long and based on the same concept. By the pin-hole geometry wave vector numbers  $Q$  between  $10^{-3}$  to  $0.3 \text{ \AA}^{-1}$  become accessible, and so mesoscopic structures between 10 and 1000  $\text{\AA}$  can be studied. The structures studied are varied, ranging from precipitates or pores in metallic alloys, polymers in solution or melts through to micelles and microemulsions.

At FRM II the combination of high neutron flux supplied by the cold neutron source, the newly designed neutron guide system, and a new collimation system allowing a larger experimental flexibility support the current major upgrade of both instruments that finally will optimize KWS-1 and KWS-2 towards particular scientific topics: KWS-1 will be a dedicated SANS diffractometer to high-resolution / grazing incidence / polarization analysis looking at thin films and hard matter systems, while KWS-2 is optimized for high intensity / wide  $Q$ -range studies of soft matter and biological systems.

Upgrades of KWS-1 and KWS-2 will include:  $\text{MgF}_2$  neutron lenses which allow for higher intensities and/or lower wave vectors  $Q$ . Thus a high resolution detector is added at a larger distance of 17m. In this configuration up to  $\mu\text{m}$  large structures can be resolved. A combination of the velocity selector with a double disc

chopper allows for higher wavelength spreads down to 1%. The pulsed neutron beam can also be used to resolve structural changes in the ms regime. The high intensity of FRM II and the new detector electronics allow for count rates of  $6 \times 10^5$  neutrons/s and will enable the studies of fast kinetics.

The investigation of structures and morphologies on wide length scale and of fast structural changes in soft condensed matter and biological systems will represent the major tasks of the KWS-2 instrument. Polymer effects on microemulsions, diesel fuels, and mineralization of inorganic compounds, thermal composition fluctuations in polymer blends and diblock copolymers, their aggregation behavior and response on shear, the rubberelasticity and the "living anionic polymerisation", denaturation of proteins by chemical agents or changes of physical parameters (temperature, pressure, etc), structural changes due to fast kinetic processes (in the ms and s range) are usually studied.

One research topic handled by KWS-2 is microemulsions. Microemulsions are macroscopically homogeneous mixtures of water, oil and surfactant. On a microscopic level, the mixtures are structured into water-rich and oil-rich domains separated by an amphiphilic film. Microemulsions have many commercial

and industrial applications (cosmetics, polishes and cleaners, detergents, pesticides) and there is an increased interest in using them as a method of synthesising nanoparticles (templates). By variation of physical parameters like temperature, composition, salinity, etc., the internal domain structure can be varied. One finds for instance globular or cylindrical droplets, which can be disordered or ordered in the liquid crystalline phase. The majority component usually hosts well separated domains, except for the bi-continuous phase where each domain has a sponge like structure.

Figure 1 presents the small angle scattering patterns from an oil in water microemulsion with the non-ionic surfactant Igepal-CO520. A transition from a mixture of spherical and cylindrical droplets to long flexible cylindrical structures is observed upon decreasing temperature. The diameter and length of the elongated droplets have been accessed in this experiment. By contrast variation the film scattering could be separated from the domain scattering.

In the frame of the study of biological molecules, SANS is a suitable method to investigate the denaturated state of proteins. From a fundamental point of view, the technique will allow us to understand how a protein adopts its final conformation from its primary structure. From an industrial point of view, SANS brings answers to questions concerning the influence of physical and chemical parameters (tem-

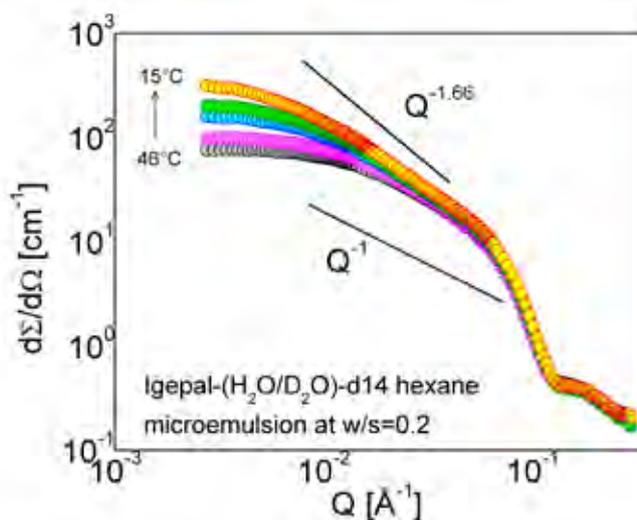


Fig.1: SANS patterns from a microemulsion system collected at different temperatures.

perature, pressure, pH, ionic strength, etc.) on biological molecules, of an essential importance in food industry (sterilization and bio-conservation). In medicine, degenerative diseases such as Alzheimer or Parkinson involve slightly unfolded proteins around brain receptors leading to the typical symptoms of memory loss or even malfunction of muscle coordination. Recent and promising results have shown that it is possible to investigate different folding states of a model protein, the horse heart myoglobin, by using chemical denaturing agents (guanidinium hydrochloride).

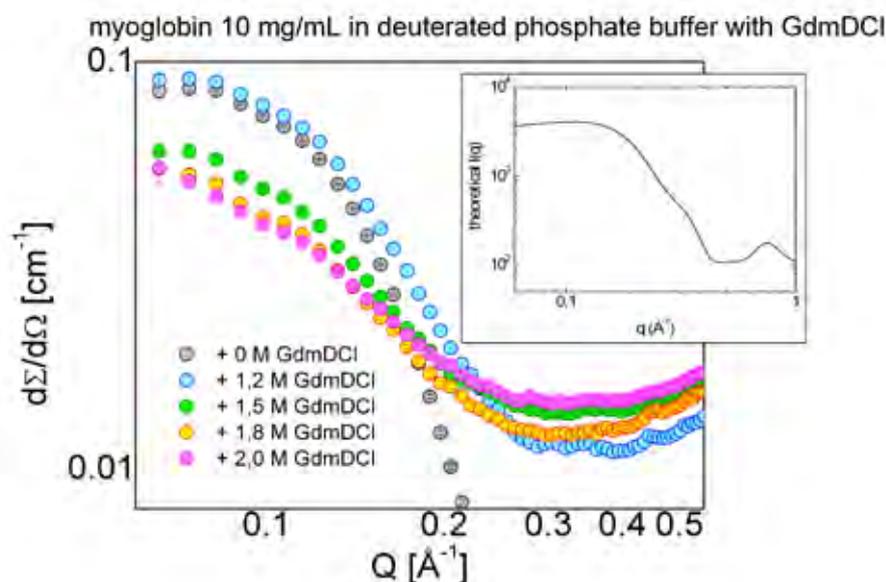


Fig.2: SANS patterns from a myoglobin protein in buffer solution for different amount of denaturing agent added. (In the courtesy of M.-S. Appavou)

Figure 2 shows in a Kratky representation the small angle scattering patterns from myoglobin protein in phosphate buffer for different concentrations of denaturing agent added. In the absence of the denaturing agent the protein is in its native globular state. When the denaturing agent is added the molecule starts to unfold showing an expanded globular shape (for 1.2M GdmDCI added) and shows the scattering features of an unfolded molecule (above 1.5M GdmDCI added).

## Focussing Neutrons at a Point: Improving Flux and Resolution by a Focussing Supermirror Guide at RESI

For modern neutron single crystal diffractometers using area detectors to image reciprocal space the crystal size is one of the limiting factors: using larger crystals in order to obtain a higher signal typically leads to an increased spot size on the detector deteriorating the resolution. In the ongoing optimization process of the instrument RESI recently a major step to overcome this paradigm has been achieved installing a semi-elliptical supermirror guide focussing onto the detector position.

The progress in the production of high quality elliptical supermirror guides with values of  $m$  up to 5 allows us to focus the neutron beam to give significantly smaller spot sizes. Focussing the neutron beam onto the crystal results in an improved flux at the sample, but at the cost of a comparably large spot on the detector giving worse resolution. Another idea is to focus instead onto the detector. This still results in some flux increase at the sample position, but the major benefit is an improved resolution and an increased signal/noise ratio on the detector (you will get more neutrons per pixel).

Fig. 2: Focussing guide of RESI.

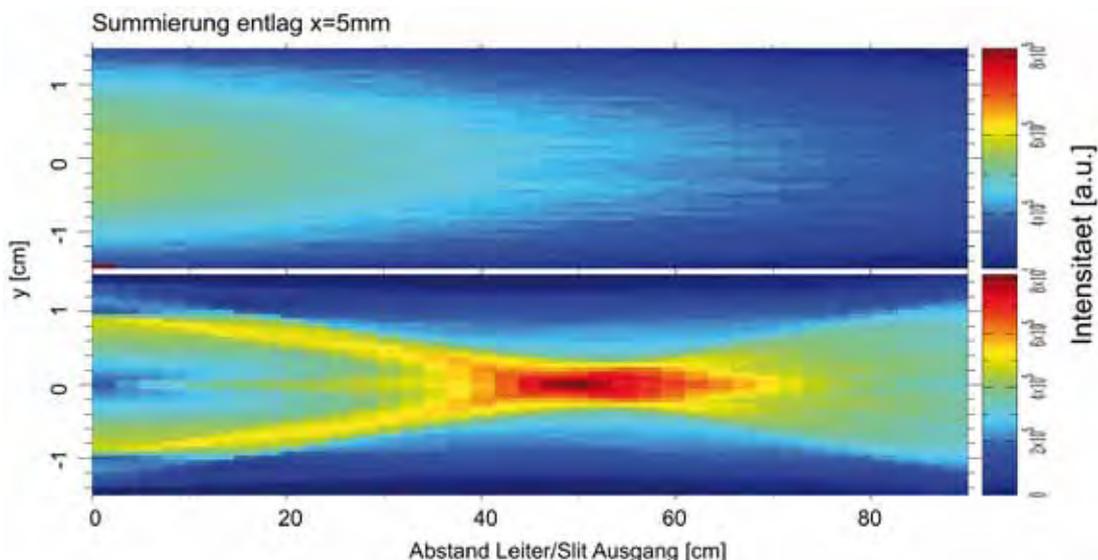


Fig. 1: Monte Carlo simulation of intensity distribution of focussing guide.

To test this idea neutron ray-tracing calculations with McStas (A. Ostermann) have been performed, showing that a channeled focusing guide can give a focal point 500 mm from the guide exit, if using  $m$  greater than 5 (see figure 1). The final design chosen is a semi-elliptical guide element of 1m length with an inner channel (see. figure 2) with  $m=5$  coating for the upper and lower mirrors. This guide element has a focal distance of 500 mm from the guide exit. The left and right side walls were kept uncoated to avoid an increase of the horizontal divergence. Manufactured by SwissNeutronics the guide was installed on RESI during the February shutdown (see figure 2). A translation unit allows a reproducible installation of the guide within a very short time.

First tests during the alignment confirmed the very good focussing properties of the guide element. The focal spot was found to be within 5mm of the theoretical position, confirming the high quality of the mirrors. Comparative measurements on a standard sample finally confirmed a gain in usable intensity on the detector of almost 2 for a wavelength of 1.5 Å. Although the focusing effect is much smaller for 1 Å neutrons, due to the better beam shielding by the boron float glass, the guide still reduces the background considerably yielding an improved signal to noise ratio.

Bjørn Pedersen  
FRM II

## Tunneling, Relaxing, Diffusing. The Back-Scattering Spectrometer SPHERES

Forty years after the first demonstration of principle, backscattering is back to Garching. Built and operated by Forschungszentrum Jülich, SPHERES (**SP**ectrometer for **H**igh **E**nergy **RES**olution) is a third-generation backscattering spectrometer with focussing optics and a phase-space transforming chopper. It went into regular user operation in the course of 2008. Sadly, the completion of the instrument was clouded by the sudden death of its long-term scientific advisor, Michael Prager.

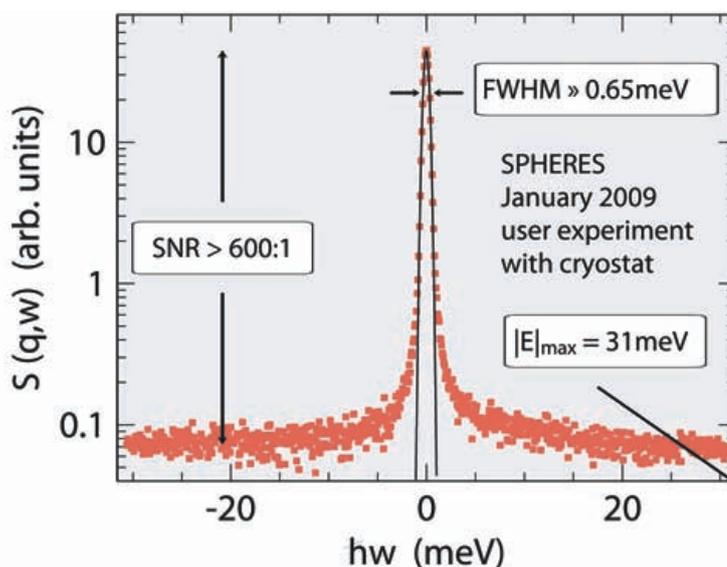
In the Si(111) standard configuration, SPHERES has an excellent energy resolution of 0.62 to 0.65  $\mu$  eV, and an energy range of  $\pm 31 \mu$  eV. Other parameters, especially the flux ( $8 \cdot 10^5 \text{ s}^{-1}$  at the sample) and the signal-to-noise ratio (600:1 under realistic conditions, with user-provided samples), confirm that SPHERES is one of the leading instruments of its kind.

In 2008, eight external user groups were served. In 2009, the same number was already reached in May. Several experiments were performed in the most classical domains of backscattering spectroscopy: hyperfine interactions and rotational tunneling. Apart from these special applications, SPHERES is mostly used for broad-band spectroscopy on diffusional or relaxational dynamics. As a multidetector instrument with relaxed Q resolution (Q range: 0.6-1.8  $\text{\AA}^{-1}$ ; 0.2-0.6  $\text{\AA}^{-1}$  with reduced energy resolution;  $\Delta Q \approx 0.1 \text{\AA}^{-1}$ ), SPHERES is particularly suited for measuring incoherent scattering (typically from hydrogen). Insofar, it is complementary to neutron spin echo.

Traditionally, backscattering instruments have often been used for elastic temperature scans. Given the high flux at SPHERES, it is now also possible to perform *inelastic* temperature scans. Every few minutes, we save a spectrum, and later, we integrate over appropriate energy intervals, or we fit a simple model. It can be shown that the so obtained inelastic temperature ramp, though a hundred times weaker than the elastic signal, may contain the more valuable information; in this case, it clearly reveals a phase transition.



Watching the S(111) analyzers. Joachim Wuttke, Gerald Johannes Schneider and Luis Carlos Pardo Soto of SPHERES.



Joachim Wuttke  
JCNS, Garching

SPHERES instrumental resolution.

## Development of High m Supermirrors at the Neutron Optics Group at FRM II

With increasing demand for neutron guides of higher glancing angles the neutron optics group of FRM II started to optimize the existing sputtering machine in order to produce supermirrors with higher m values. The group has now been able to improve the sputtering process for the production of supermirrors with  $m=3$  and  $m=3.5$ . Before only supermirrors with glancing angles of up to  $m=2.5$  as standard could be produced. These Ni/Ti supermirrors have been successfully used to produce neutron guides mounted at FRM II and at several other facilities.

### m=3 supermirrors

In order to achieve high reflectivity at large angles it is necessary to grow multilayers with low roughness and interdiffusion at Ni/Ti interfaces. The major problem with these large m mirrors is the fact that with increasing thickness the force acting from the coating on the substrate exceeds the mechanical strength of the glass and gives rise to fractures, leading even to coatings coming away from the substrate surface.

Aiming to minimise the roughness of the individual layers as well as the interface roughness and to prevent the interdiffusion among layers we introduced an additional gas such as nitrogen or dry air during the sputtering of Ni (reactive sputtering). With this new setup it was possible to optimize the sputtering process for the production of supermirrors with  $m=3$ . The results show a reflectivity higher than 85% (edge value). This competes with other commercially available products. Our multilayers show a very good adhesion to borofloat glass. Also the deposition process itself is very stable.



The FRM II's neutron optics group.

### m=3.5 supermirrors

With increasing experience with reactively sputtered supermirrors we started the next step to go to  $m=3.5$ . In this system the number of layers grows from below 500 (as for  $m=3$  supermirrors) to nearly 700. This drastic increase is expected to lead to higher intrinsic stress and lower adhesion. Therefore extensive studies were necessary to build a layer system which combines high reflectivity and adequate mechanical stability. Finally an optimized layer system has been found. At  $m=3.5$  reflectivity values around 81% were reached, which is the actual state of the art. The process proved to be stable (see figure 1).

In the near future we plan to start production of nonmagnetic supermirrors. Besides, we study the effect of additional Cr layers on neutron optical properties of the mirrors. These Cr layers are expected to lead to a decrease of roughness and a better adhesion of the first Ni layer to the substrate and therefore to a better stability of the stack. In addition, the development of supermirrors with higher m will be continued by increasing accordingly the number of layers.

Gunther Borchert  
FRM II

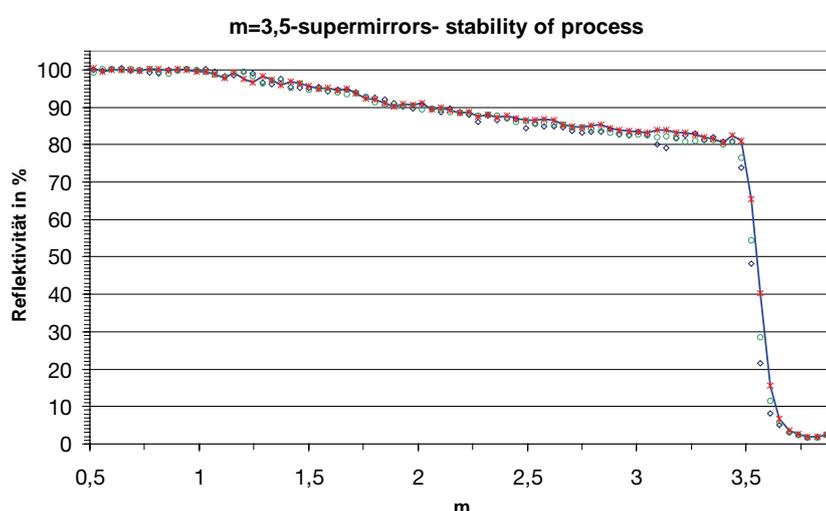


Fig. 1 The reflection curves of several  $m=3.5$  supermirrors produced in different processes exhibit only minor variations.

## 2<sup>nd</sup> User Meeting at FRM II May 25, 2009 - Garching



Happy users and staff of the FRM II on a wonderful summer day.

A warm summer day brought together over 130 users and members of FRM II for the 2<sup>nd</sup> FRM II User Meeting. It was held at the Faculty of Physics of Ludwig Maximilians-Universität München (LMU) and the Department of Physics of Technische Universität München (TUM) in Garching. In a very friendly atmosphere at the Faculty of Physics of LMU users gave talks on experiments performed recently at FRM II. These were well received and discussed by the audience, in the full lecture hall. Oral presentations and posters dealt with the fields of *Instrument and Methods, Magnetism and Dynamics, Material Science, Soft Matter and Particle Physics*, spanning the broad option for science at the instruments at FRM II.

In the *Instruments and Methods* section an interesting and colourful oral presentation was given by Michael Schulz of TUM, demonstrating the option of polarised neutron radiography available at ANTARES to study concentration fluctuation in single crystals of ferromagnets. Neutron radiography at the NECTAR facility was used by Kurt Osterloh of BAM in Berlin in his study of heterogeneities and damages in wood. Another captivating study using neutron radiography was presented by Helen Hermes of Heinrich Heine University of Düsseldorf, in her investigation of the dissolution of amphiphiles by time- and space resolved neutron imaging. This and various poster presentations showed the broad range of applications neutron radiography can be used for.

In the classical field of neutron investigations of magnetism Niels Christensen of Risø National Laboratory described new work on magnetic field induced soft mode quantum phase transition in high-temperature

superconductors and Nikolay Tsyrlin of ETH Zurich showed results on magnetic excitations of two-dimensional weakly frustrated  $S=1/2$  antiferromagnets. Both experiments were performed at the three axis spectrometer PANDA.

Investigations studying the structure and the dynamics in polymers and microemulsions were explained by Thomas Hellweg of University of Bayreuth on the dynamics of sugar surfactant based microemulsions using neutron spin echo spectroscopy at the instrument J-NSE of JCNS. While Joseph Adelsberger of TUM utilised small angle neutron scattering at KWS-2 of JCNS and NSE in his work on thermo-responsive block co-polymer gels.

More than 70 poster presentations gave an impressive and vivid overview of the broad range of scientific topics tackled at the instruments available at FRM II. Neutron diffraction, spectroscopy, reflectometry, small angle scattering and tomography are used by most scientists in their work, but neutron radiography, prompt gamma activation analysis and the positron facility at FRM II also get increasing use and are accepted by the scientific community. The evening poster session at the foyer of the Department of Physics of TUM with Bavarian fingerfood and beer was a real summer special with lively scientific discussions and get-togethers of users and FRM II staff members.

With the positive response of the users to the User Meeting the FRM II waits for the next meeting in autumn 2010.

Thomas Gutberlet  
JCNS, Garching



## 9<sup>th</sup> International Conference on Neutron Scattering May 3-7, 2009 - Knoxville, Tennessee

This year in May, Knoxville in Tennessee, USA, hosted the International Conference on Neutron Scattering. The largest neutron scattering conference world wide is held in a four-year cycle. This time, it brought together more than 600 scientists. Unfortunately many colleagues could not attend the meeting due to the world wide alarms on swine flu (H1N1) and the still difficult situation to apply for visa to the United States. Hence the majority of the participants came from the host nation.



The FRM II as well as JCNS were active supporters of the ICNS both with business booths for information on the facilities and the possibilities for experiments at FRM II.

Many posters and lectures were presented by collaborators and members of FRM II and JCNS showing the well recognized scientific activity of both institutions, which was also mentioned in the introductory talk by John Root of Chalk River Laboratories, Canada.

Besides several hundred oral presentations given in daily parallel sessions and large poster sessions each day, the keynote lectures given by experts in various fields attracted great attention of the conference participants. Particularly remarkable were the keynote lectures by Omar Yaghi, UCLA, California, on so-called reticular chemistry and by Chun Loong, Sun Yat-Sen University, China, who presented impressive plans of China to install a high flux reactor and a high flux spallation neutron source in China within the next decade. In addition various satellite events were organized including a McStas Workshop, courses on neutron imaging and several instrument specific meetings and workshops.



Many discussions were not only done during the conference, but also on the side in the evening in the restaurants and bars in downtown Knoxville. The stormy and rainy weather did not interfere with the participants' enthusiasm for meeting and discussing the widely topics. A highlight of the conference was an organized visit of the nearby Spallation Neutron Source SNS and the High Flux Isotope Reactor HFIR at Oak Ridge National Laboratory.

The conference was closed by a very humorous and relaxed lecture by Sunil Sinha from University of California, San Diego, who looked back on the development and history of neutron scattering and the tremendous future prospects by new techniques and neutron sources available for science.



In 2013, the next ICNS will be held in Europe. Three places stand for the organization of that event: Edinburgh, Grenoble and Venice. The decision will be made towards the end of the year.

Thomas Gutberlet  
JCNS, Garching

## “Hands-on Real Experiments” Fortgeschrittenen-Praktikum at FRM II

They do it voluntarily. The course is done, the credit points for their Diplom are collected. And still Linda Ahnen (20), Max Knötig (21) and Thorsten Wolf (22) listen to Dr. Robert Georgii. Fascination is in the students' eyes. They want to know more about the instrument MIRA in the neutron guide hall. What is this part for? How is the neutron spin controlled?

Linda, Max and Thorsten are students in their third year at the Physics department of the Technische Universität München. They have just finished their practical training during five days at the neutron source and handed in their experimental report. FRM II offers twice a year a “Fortgeschrittenenpraktikum”, a course for students after their first degree, the Vordiplom. Linda, Max and Thorsten talk about their experiences at the course.



Dr. Robert Georgii (left) explains to Max Knötig, Thorsten Wolf and Linda Ahnen (from left to right) the various components of the instrument MIRA.

*What other instruments did you get to use?*

*Linda:* After an introductory talk we had an experiment at the backscattering instrument SPHERES. We had to measure the rotational frequency of a methyl group.

*And what experiment did you perform at MIRA?*

*Max:* We measured the thickness of nickel on boron glass. Both experiments were very interesting.

*Thorsten:* The most important thing: These were real experiments and we could learn hands-on.

*Linda:* And we found out, that not all the experiments give the results, which were expected in the beginning.

*Why were you so fascinated about MIRA?*

*Max:* Because of the high level of science. The MIRA group has just had a publication in science, and the basics of it, the skyrmions, were discovered at MIRA.

*Thorsten:* It was also fascinating to be able to work at a large-scale research facility.

*Linda:* I also liked the guided tour through the FRM II, especially the look into the reactor pool.

*Did you get good remarks on your protocol about your practical training?*

*Linda:* There are no marks. But we got an extra little star for our 10 pages of text and graphs from SPHERES and good remarks from MIRA for another 10 pages.

*Max:* The feed-back from the instrument scientists was very positive and helpful for us. Now we know what to change next time.

*Thorsten:* The resolution of one of our graphs could have been better.

*Did you choose the course at FRM II voluntarily or is it an obligatory course for students in physics?*

*Thorsten:* The course at the neutron source is a compulsory optional practical training. We have about 40 practical courses, from which we can choose 12.

*Linda:* The FRM II practical training is very popular. One has to be fast in registration to be one of the 30 lucky students.

*Will you come back to the neutron source, maybe as a student trainee or for your theses?*

*Linda:* Right now, I am working for another institute as student trainee, but if I get an offer here – who knows?

*Thorsten:* Maybe later.

*Max:* I would be interested in a diploma thesis, but it is too early now to decide.

Andrea Voit  
FRM II



### NMI3 - 2.2 Mio € EU-Funding for Neutrons

March 30-31, 2009 - Villigen



In the middle of the participants of the kick-off meeting at PSI: Helmut Schober (ILL), the project coordinator.

On February 1<sup>st</sup>, 2009, the new "Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy" (NMI3), which combines 23 partners in 14 countries was started. FRM II and JCNS both are members of the NMI3 consortium together with ten other European neutron and muon research centres and a number of European research institutions and universities. The official kick-off meeting of the new NMI3 project was held on March 30-31, 2009, at PSI, Villigen, Switzerland.

The aim of NMI3 is the pan-European co-ordination of neutron scattering and muon spectroscopy, supporting these research infrastructures as an integral part of the European research area. Co-ordination and networking within NMI3 will lead to a more strategic approach to future developments and thus re-inforce European competitiveness in this area.

The following activities and tools are implemented within NMI3:

- Transnational ACCESS will be provided by 10 partners offering more than 4000 days of beam time. FRM II and JCNS both participate in the ACCESS program giving European users access to all European infrastructures and hence the possibility to use the best adapted infrastructure for their research. Travel costs and accommodation for European users to experiments are covered by the ACCESS program.
- Joint Research Activities (JRA) focusing on six specific R&D areas will develop techniques and methods for next generation instrumentation. They involve all those European facilities and academic institutions with major parts of the relevant know-how.

- Dissemination and training actions will help to enhance and to structure future generations of users.
- Networking and common management will help strategic decision-making from a European perspective.

The total funding by FP7 for NMI3 amounts to nearly 10 million euros. From this the FRM II and JCNS will receive a total of 2.2 million euros over the four years of the project. Most of the funding provides free access for European scientists to the FRM II and JCNS to perform their experiments with neutrons.

More than one million Euros are reserved for new projects in the field of detector development, sample environment, muons, neutron polarization, deuteration facilities and neutron optics. For example new mirrors for neutron guides are constructed by the Technische Universität München, while JCNS will investigate aspherical lenses for beam focusing for SANS. JCNS is the lead laboratory of the neutron polarization activities and participates also in the detector development and neutron optics. The JRA on new detector development is lead by the FRM II detector group. In collaboration with the Department of Chemistry of TUM segmental labeling of biomolecules will be developed in the Deuteration JRA.

The ACCESS program of NMI3 will give support only for the next two years and will come to an end in January 2011. The JRA activities will be active for four years till the end of the NMI3 funding period in January 2013.

Thomas Gutberlet  
JCNS, Garching

## Evolving Stress during Casting: In situ Experiments at STRESS-SPEC

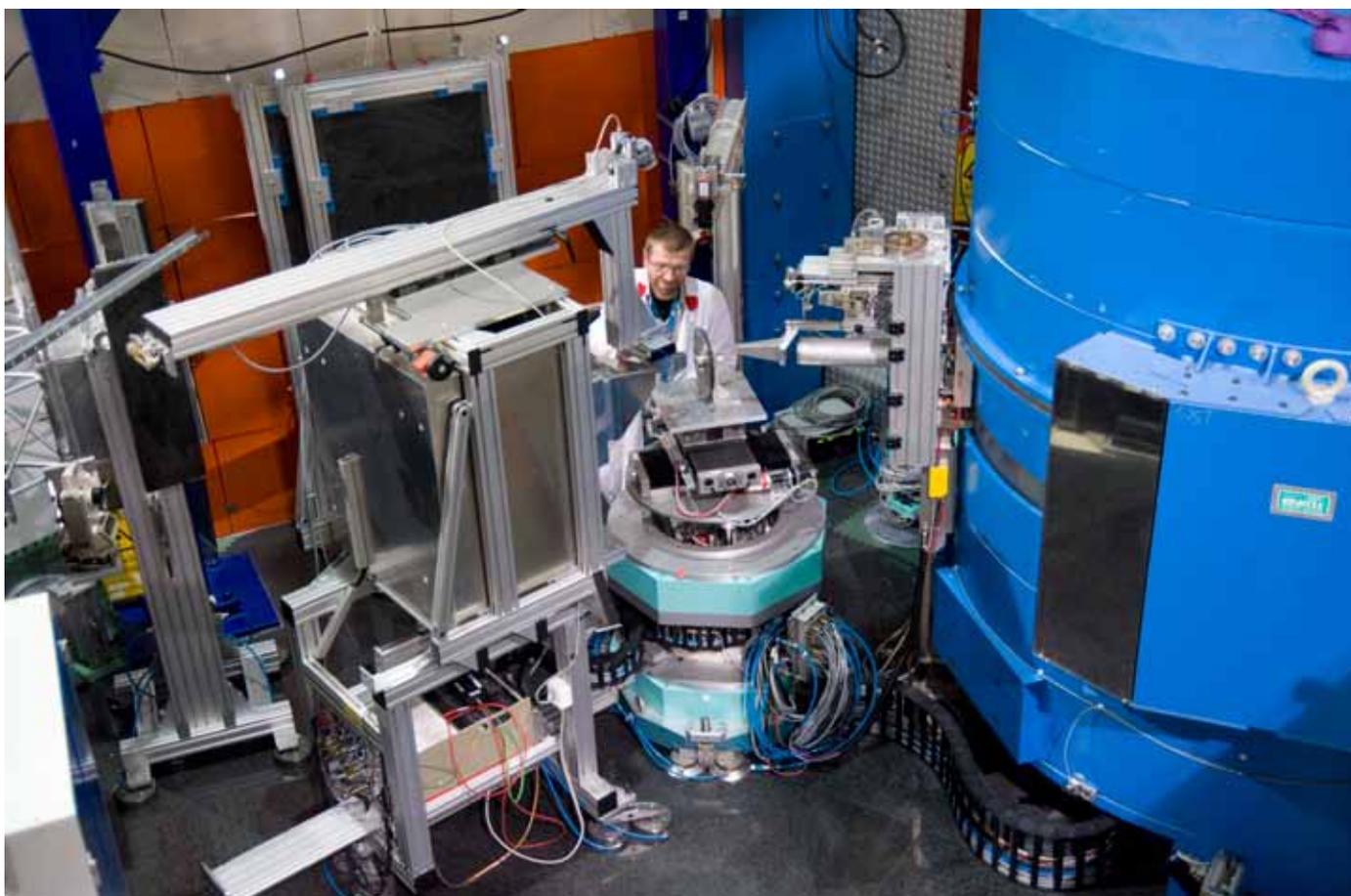
Enhanced links with the Engineering Departments of the Technische Universität München and the FRM II material science diffractometer STRESS-SPEC resulted in several joint DFG funded research projects. The two partners, the Department of Metal Forming and Casting (Lehrstuhl für Umformtechnik und Gießereiwesen, utg) and the Institute of Materials Science and Mechanics of Materials (Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, wkm) collaborate closely with the neutron source.

As an example for these successful collaborations we outline here some of the key aspects emerging from our studies on the development and simulation of residual stresses in aluminium composite castings. The project was conducted by Uwe Wasmuth (utg) in his Ph.D. thesis. The ability to carry out in situ strain measurements has proved central to the project's success.

In the course of the thesis, significant discrepancies have been found between the experimentally determined data and numerical models obtained by standard finite element modelling (FEM) of casting processes. These discrepancies were attributed to relaxation

processes at high temperature and during cooling of the aluminium cast.

As stress relaxation effects are difficult to determine experimentally at high temperatures with conventional techniques, by using neutron diffraction we were able to carry out in situ strain measurements during the solidification process of the aluminium cast of the test specimen. The *in situ* neutron experiments were carried out on the diffractometer STRESS-SPEC during the cool down of a composite cast test specimen (steel ring insert and outer aluminium cast) after casting aluminium in a single sand casting mould installed on the sample table (figure 1). A great advantage is that this experiment allows the processes to be monitored during real-time cooling of the sample. All diffraction data were taken in the hoop strain direction of the steel insert. The measurements were started approximately two minutes after a cast temperature of  $T = 550^{\circ}\text{C}$  was reached in the aluminium melt ("semi-liquid" region). The count time of the measurements was 60 seconds per point. The thermal expansion of the steel was measured separately in the same experimental configuration and subtracted from the diffraction data, thus allowing the mechanical strain to be obtained.



Instrument scientist Michael Hofmann at STRESS-SPEC.

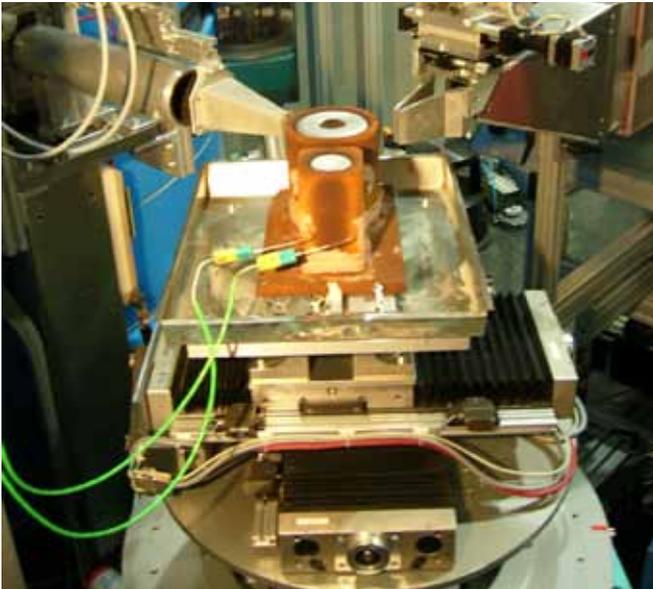


Fig. 1: Sand mould after casting the aluminium on the sample table.

Figure 2 shows the onset of the build up of compressive mechanical strain at about 350°C as the sample cools. At higher temperatures the aluminium is in the plastic regime due to relaxation effects and the low values of the high temperature strength. At temperatures below  $T \sim 150^\circ\text{C}$  no further increase of mechanical strains is found as the yield point of aluminium is exceeded locally within the aluminium cast.

As also shown in figure 2, the residual stresses calculated from the experimentally determined strains differ considerably from the results of a time independent numerical simulation – an elastic-plastic simulation as implemented in standard FEM casting routines. In fact the values of the numerical simulation are 3 times as large in magnitude for steel and for aluminium. These discrepancies in the simulation are attributed to use of the standard, time independent model for the casting alloy and indicate that extension of the standard model is required. The

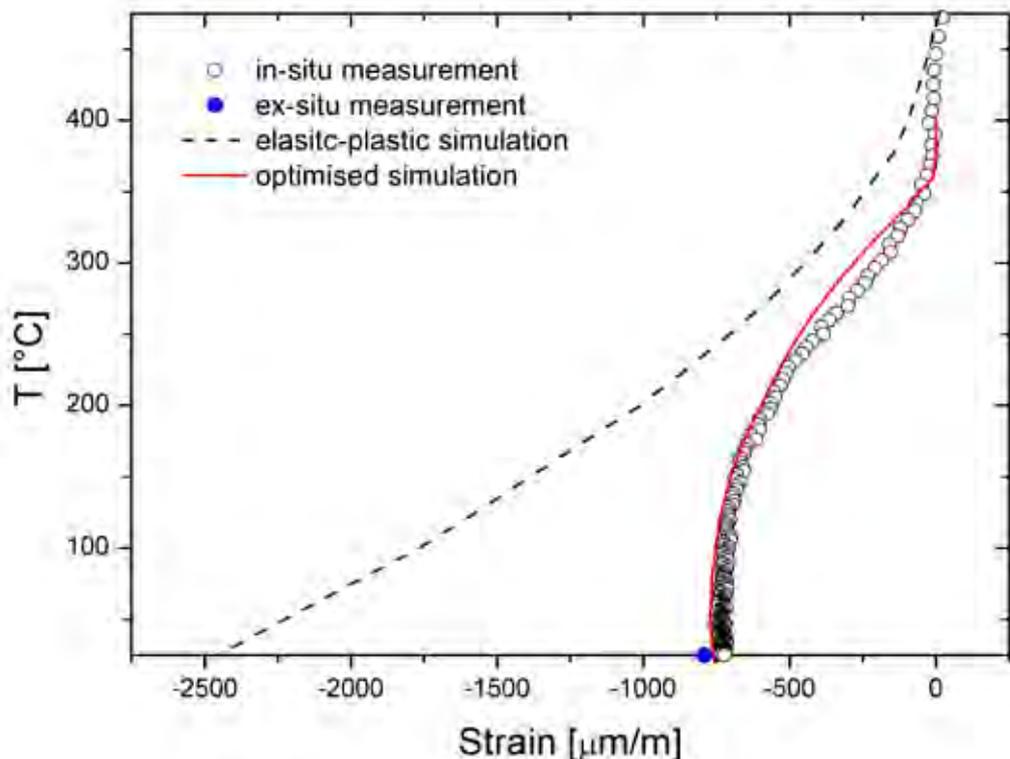
standard time independent simulation overestimates the elastic strain in the aluminium cast.

Based on these experimental findings and the poor agreement of experimental results with simulations using the standard time independent model, assuming that stress relaxation processes, like creep, occur during the solidification of the aluminium cast, a time and temperature dependent material model was developed and included in the standard model. Figure 2 shows the excellent agreement of this extended numerical simulation with the experimental data and the results of an earlier ambient temperature experiments.

We are confident that these experimental results could be used to verify universal relaxation models in casting simulations and therefore we have already initiated an extension of this successful DFG project to investigate this behaviour in detail. In addition further applications have been submitted to the DFG to study phase kinetics in cast iron alloys (together with utg), as well as high temperature behaviour of superalloys under deformation (together with wkm).

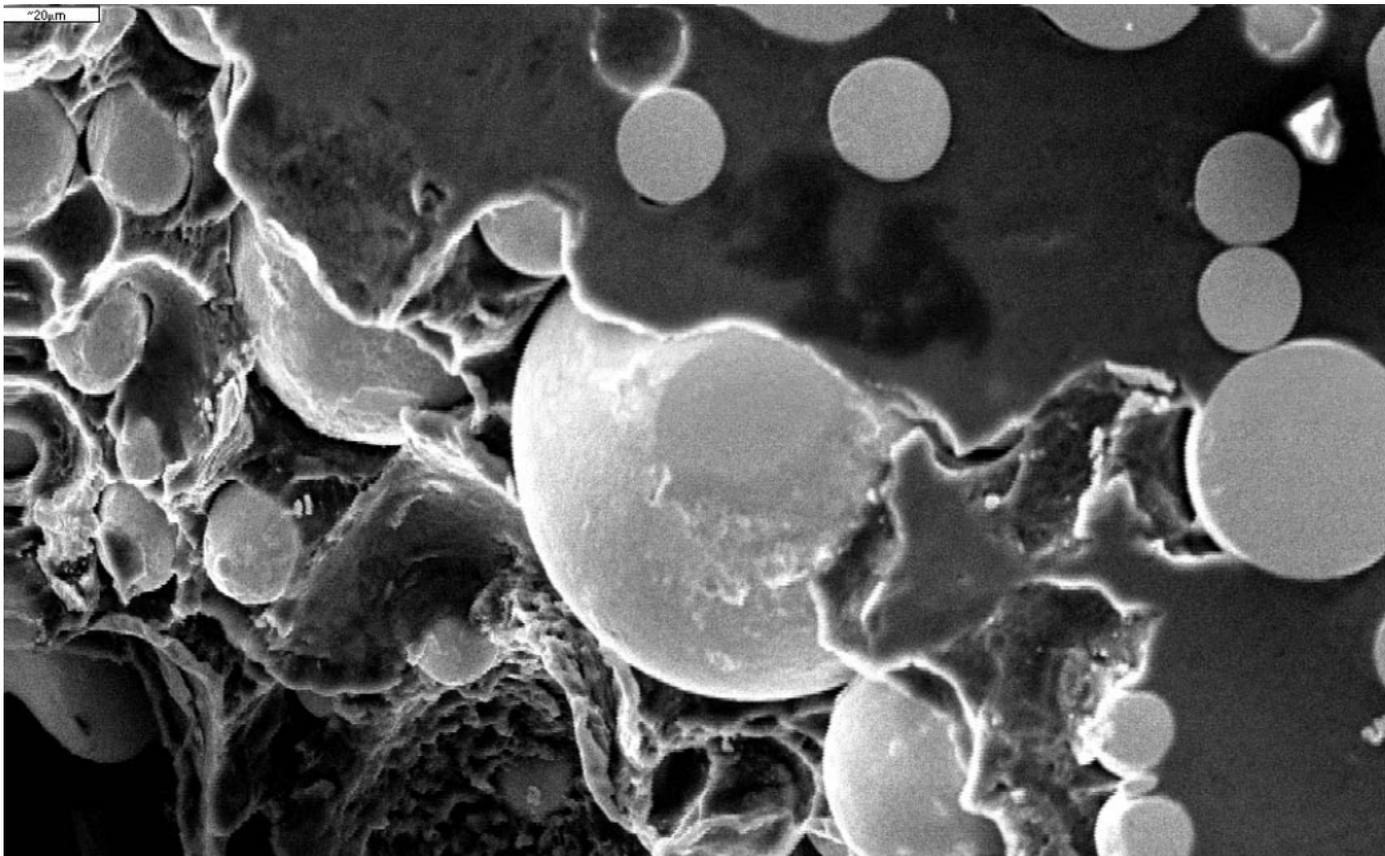
Michael Hofmann  
FRM II

Fig. 2: Values of the extracted mechanical hoop strain together with results for the time independent simulation (dotted line) as well as the optimised, time dependent simulation (red line). The blue data point marks the result of an ambient temperature experiment.



## From HEU to MEU

### Developing new Materials for the Fuel Element of FRM II



A scanning electron microscope picture of a cut-through disperse sample with Uranium-Molybdenum and aluminium.

Rainer Jungwirth has to choose from 20 different candidates. Each of them is put to the acid test. In the end, only one can succeed and will go to Belgium within the next two years. The candidates are the size of a finger nail and are made of depleted uranium as well as a different mixture of aluminium. Rainer Jungwirth examines new material combinations for the development of a new fuel element for the FRM II reactor core. As part of its operating license, the Technische Universität München (TUM) has to manage the conversion of the fuel element from highly enriched uranium (HEU) with up to 93 percent of the fissionable  $^{235}\text{U}$  to medium enriched Uranium (MEU) below 50 percent of  $^{235}\text{U}$ . To achieve this goal without penalizing the neutron flux, the density of uranium in the fuel element of FRM II has to be increased. There are generally two different sorts of material thought to be suitable for fuel plates with higher densities: monolithic Uranium-molybdenum with densities of Uranium up to  $16 \text{ g/cm}^3$  and Uranium-Molybdenum in powder form with densities up to  $8 \text{ g/cm}^3$ .

At the FRM II a research group of 6 scientists works on the development of this new fuel. Rainer Jungwirth

tests the different materials by bombarding them with heavy ions on the Maier-Leibnitz-Laboratorium, a tandem accelerator of the TUM and Ludwig-Maximilians-Universität München. Up to now, a so-called interdiffusion layer has prohibited the successful development of an adequate new fuel element with lower enrichment of  $^{235}\text{U}$ . The interdiffusion layer (IDL) forms under irradiation at the interface of the grain made of Uranium-Molybdenum and the matrix of the fuel plate made of aluminium. In the end, the interdiffusion layer can result in a burst of the fuel plates. This happened to LEU-plates with higher density of  $^{235}\text{U}$  developed in the US and in France in 2004. The research group of FRM II tested a little later its own Uranium plates, which only swelled, but did not burst. So the goal of Rainer Jungwirth is to find out, what material compositions can prevent the development of the IDL. He examines the tested mini plates with x-ray diffraction, optical and scanning electron microscopy. The successful material is foreseen to undergo irradiation testing at the Belgian material test reactor BR-2 at Mol and be examined in there afterwards. With the "Centre d'Energie Atomique" in France, there is a close exchange of experiences.



Wolfgang Schmid with the prototype sputtering plant for the first test production of the newly developed plates.

While Rainer Jungwirth is screening the candidates, Wolfgang Schmid is developing a method to create the new fuel plates in close collaboration with the fuel plate manufacturer Areva NP subsidiary Cerca. In parallel to irradiation tests of different alloys of monolithic Uranium-Molybdenum (UMo) of lower enrichment an industrial fabrication process for these alloys has to be established. “The first challenge is to bring the fuel alloy into the desired plate shape. The second is to install a barrier, which prevents diffusion. The third and final challenge is to surround everything with the aluminium cladding“, says Schmid.

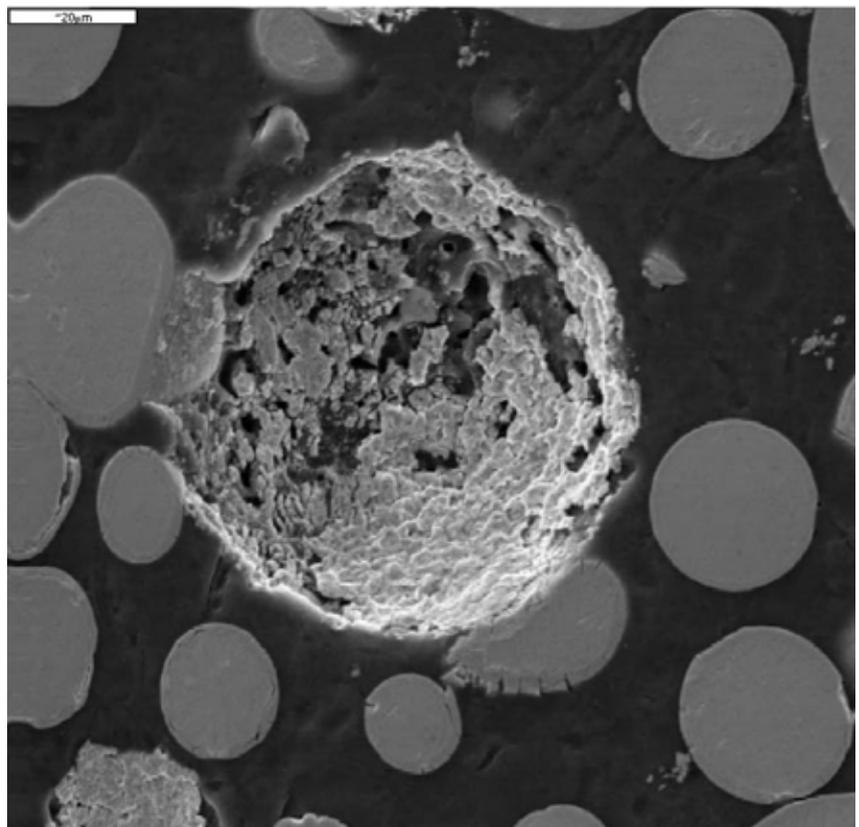
Each manufacturing step is important, because many UMo alloys have adverse material properties that make any processing difficult. Most conventional manufacturing techniques completely fail for UMo alloys, the few remaining are not efficient. Schmid wants to use the sputtering technique as an alternative. “Sputtering allows us to build up a full-sized reactor fuel plate atom by atom. In this way we avoid all the manufacturing problems caused by the adverse material properties of the UMo. The resulting structures are superior to conventionally manufactured fuel plates. But it takes a lot more time to sputter a plate“, Schmid points out. First experiments showed that a production of UMo foils in the desired thickness and the installation of barrier and cladding layers is easily possible by sputtering. “Now we have to increase the foil

size by a factor of 10 to get full size plates“, says Schmid. For this purpose a prototype sputtering plant for the production of full size plates has been built and the first production tests are in preparation.

Another important part of the conversion studies are the calculations of the neutronics and thermohydraulics, which are conducted by Harald Breittkreutz and Anton Röhrmoser, who already did the design calculations for the current fuel element. As a premise, the existing outer geometry of the fuel element of FRM II with higher Uranium density has to stay unchanged. Another important limitation is the flux of neutrons, which may only be diminished marginally. Deterministic as well as Monte Carlo methods of calculations are used for neutronics. “In a figurative sense, we follow the paths of the neutrons that leave the fuel element and look what happens to them“, says the physicist Harald Breittkreutz. He uses a brand new computational fluid dynamics code to calculate cooling conditions of the fuel element and compares them with results of the more classical methods. “The power density in the core, which is necessary for any cooling calculation, is another result of pursuing the neutron ways“, says Anton Röhrmoser.

Andrea Voit  
FRM II

The white round structure in the middle shows the oxid layer of a Uranium-Molybdenum particle, that was cut out, when preparing the sample for the scanning electron microscopic picture.



## Newly Arrived at FRM II

### Giovanna Giulia Simeoni



*What are you doing at the FRM II?*

I am co-instrument scientist at TOFTOF.

*What have you done before?*

I did my PhD at the University of Rome *La Sapienza*.

*What are your special scientific interests?*

Phase transitions in complex systems and interplay between magnetic properties and structural changes induced in multiferroic materials and other strongly correlated electronic systems.

**Contact:**

Phone: +49.(0)89.289.14975

Email: [giovanna.simeoni@frm2.tum.de](mailto:giovanna.simeoni@frm2.tum.de)

### Wouter Borghols



*What are you doing at the FRM II?*

I am second beamline scientist at DNS.

*What have you done before?*

I worked at the Delft University of Technology in the Netherlands.

*What are your special scientific interests?*

Exploring the field of nanoscale magnetism.

**Contact:**

Phone: +49.(0)89.289.10716

Email: [w.borghols@fz-juelich.de](mailto:w.borghols@fz-juelich.de)

### Enrico Faulhaber



*What are you doing at the FRM II?*

I am second instrument scientist at PANDA-spectrometer.

*What have you done before?*

I worked at the University of Technology in Dresden after finishing my PhD there.

*What are your special scientific interests?*

Interaction of superconductivity and magnetism, also improving the in-situ measurements under extreme conditions (low temperature, high magnetic fields).

**Contact:**

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Email: [enrico.faulhaber@frm2.tum.de](mailto:enrico.faulhaber@frm2.tum.de)

### Weimin Gan



*What are you doing at the FRM II?*

I am co-scientist at STRESS-SPEC.

*What have you done before?*

I did my PhD at the Clausthal University of Technology.

*What are your special scientific interests?*

Texture investigations in light weight Al and Mg alloys.

**Contact:**

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Email: [weimin.gan@gkss.de](mailto:weimin.gan@gkss.de)



## New User Office Homepage: [www.frm2.tum.de/en/start](http://www.frm2.tum.de/en/start)

After an extensive gathering of suggestions for improvement, the new homepage of the FRM II User Office has finally gone online!

The new web entrance welcomes the user by a fresh and tidy new style. The navigation is intuitive with pictures to help find one's way:

„**News & Dates**“ will keep you informed about latest news and important dates like upcoming deadlines for the submission of proposals.



The „**User Guide**“ tries to answer all of the users' questions before they have to ask them. It is divided in four parts: A „**Workflow Description**“ gives a summary of the whole course of events from the registration as a user at FRM II to the notification of a publication. A checklist can be downloaded – with it, you won't forget anything about your experiment at the FRM II! Within your user account you have to use modules. They are sometimes a little bit tricky and many users find it difficult to handle them. You find detailed explanations and instructions for each module individually in the User Guide.

Some questions are frequently asked: How to get access to the FRM II? What to prepare for the radiation protection? What requirements have to be met to obtain EU-support? You find the answers in the „**FAQ**“.



Frequently, users like to know something about the surroundings of the FRM II in advance. If you are searching for a hotel at Garching or want to know how

to arrive at the FRM II from Munich airport by public transportation, information of this kind is offered under the heading „**On Site**“.

The „**Downloads**“-area is more convenient now. For example, the .pdf-forms that are made available here can mostly be completed directly at the computer. In addition to templates to draw up proposals and experimental reports, you find the FRM II news here.



Don't be disappointed when logging in your **user account** at the FRM II! Nothing's changed. We are working on a complete new system, but that will take some time. Meanwhile we hope to improve the user-friendliness of the existing system by offering you these new help and information pages. It would be of great help getting some feedback from you. If you could not find what you need or if you have an suggestion for improvement: please send an email to the User Office!

Ina Lommatzsch  
FRM II

## Publications Archive Online

Now there is the possibility to search for released publications that are concerned with the FRM II.

On [www.frm2.tum.de/en/information/publications-archive/index.html](http://www.frm2.tum.de/en/information/publications-archive/index.html) you can use the convenient search function.

An urgent request:  
You did experiments at the FRM II, have already published about them but can't find anything in our archive? We are reliant on your active engagement in order to keep it up to date. Therefore we would be grateful if you keep your local contact at the FRM II always well informed about your publications!

Ina Lommatzsch  
FRM II

## Upcoming

### August 03-05, 2009

Polarized Neutrons and Synchrotron X-rays for Magnetism 2009 (Bonn, Germany)

[www.fz-juelich.de/iff/pnsxm2009](http://www.fz-juelich.de/iff/pnsxm2009)

### September 07-18, 2009

13. JCNS Laboratory Course: Neutron Scattering (Jülich/ Garching, Germany)

[www.fz-juelich.de/iff/wns\\_lab\\_now](http://www.fz-juelich.de/iff/wns_lab_now)

### September 13-18, 2009

SAS 2009: 14. International Conference on Small Angle Scattering (Oxford, United Kingdom)

[www.sas2009.org/](http://www.sas2009.org/)

### September 20-23, 2009

GISAS 2009: Conference on neutron and x-ray based grazing incidence small-angle scattering (Hamburg, Germany)

[indico.desy.de/conferenceDisplay.py?confId=797](http://indico.desy.de/conferenceDisplay.py?confId=797)

### September 27-29, 2009

JCNS Workshop 2009: OffSpec: Theory and Data Analysis for Grazing Incidence and Off-Specular Scattering (Feldafing, Germany)

[www.jcns.info/Workshop\\_OffSpec/](http://www.jcns.info/Workshop_OffSpec/)

### October 05-08, 2009

JCNS Workshop 2009: Trends and Perspectives in Neutron Scattering on Soft Matter (Tutzing, Germany)

[/www.jcns.info/Workshop/](http://www.jcns.info/Workshop/)

### October 24, 2009

Open Doors FRM II (Garching, Germany)

[www.frm2.tum.de/en/events/open-doors-2009/index.html](http://www.frm2.tum.de/en/events/open-doors-2009/index.html)

### November 10-13, 2009

Jülich Soft Matter Days 2009 (Bonn, Germany)

<http://www.fz-juelich.de/iff/jsmd2009>

### January 26-30, 2010

Flipper 2010: International Workshop on Single-Crystal Diffraction with Polarised Neutrons (Grenoble, France)

[www.ill.eu/news-events/workshops-events/flipper-2010](http://www.ill.eu/news-events/workshops-events/flipper-2010)

### February 24-26, 2010

SNI 2010: German Meeting for Research with Synchrotron Radiation, Neutrons and Ions on Large Scale Facilities (Berlin, Germany)

[www.sni2010.de](http://www.sni2010.de)

## Reactor Cycles FRM II 2009

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



Enjoy the Summer!

## Deadlines Proposal Rounds



FRM II (N° 10)  
July 17<sup>th</sup>, 2009  
[user.frm2.tum.de](http://user.frm2.tum.de)



JCNS (N° 6)  
September 14<sup>th</sup>, 2009  
[fzj.frm2.tum.de](http://fzj.frm2.tum.de)

## IMPRINT

### Editors

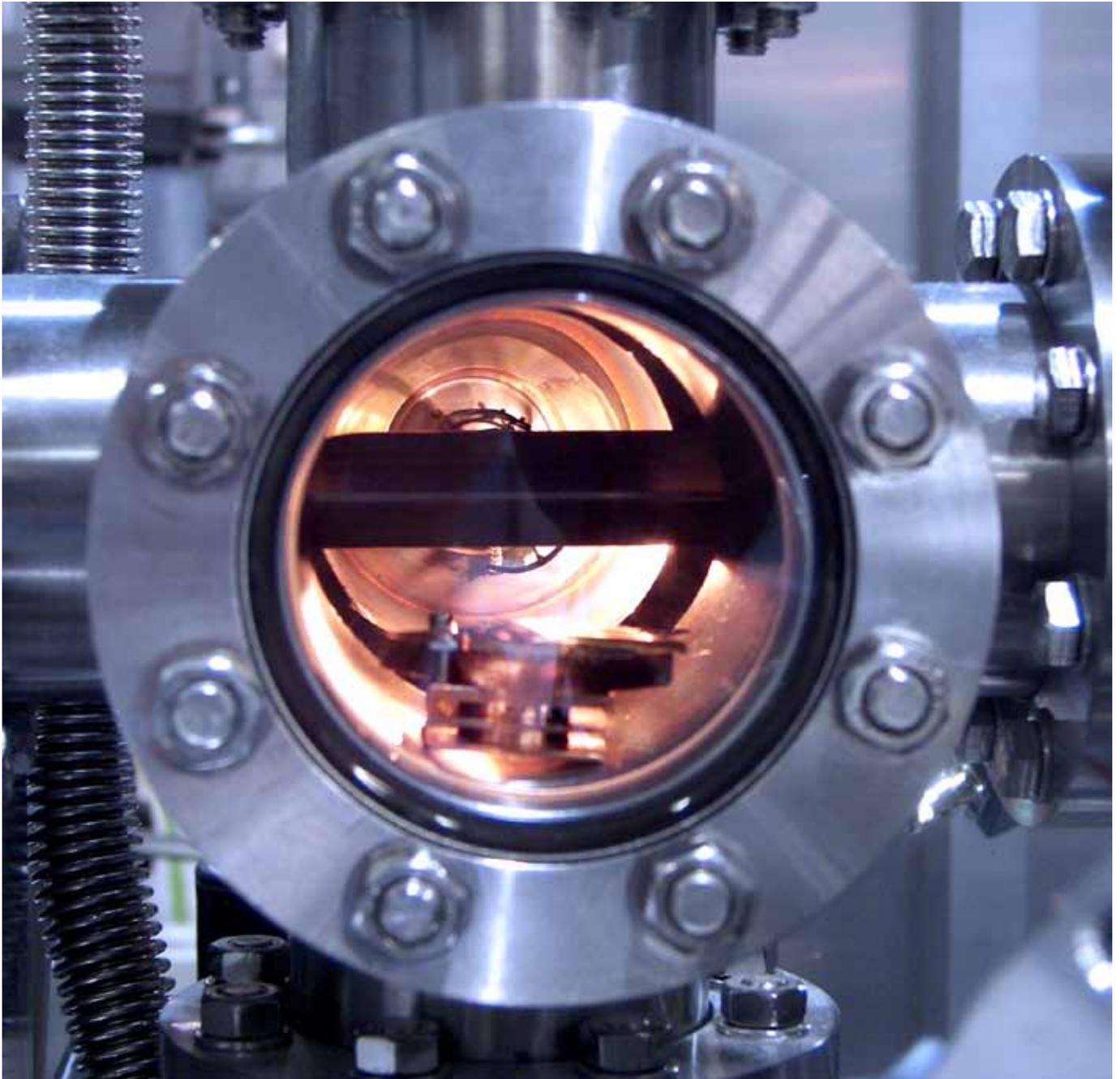
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Richard Mole  
Jürgen Neuhaus  
Andrea Voit

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[www.frm2.tum.de](http://www.frm2.tum.de)



Sewer port for samples at the positron source of FRM II.

**Light my Vacuum.**