



Newsletter

18

MLZ is a cooperation between:

The Heinz Maier-Leibnitz Zentrum (MLZ):

The Heinz Maier-Leibnitz Zentrum is a leading centre for cutting-edge research with neutrons and positrons. Operating as a user facility, the MLZ offers a unique suite of high-performance neutron scattering instruments. This cooperation involves the Technische Universität München, the Forschungszentrum Jülich and the Helmholtz-Zentrum Geesthacht. The MLZ is funded by the German Federal Ministry of Education and Research, together with the Bavarian State Ministry of Education, Science and the Arts and the partners of the cooperation.

SPONSORED BY THE

Bavarian State Ministry of
Education, Science and the Arts



Federal Ministry
of Education
and Research



The Next Big Step

An editorial by

The roots of German neutron science can be traced back to Garching and Jülich where the first research reactors started operations back in the 1950s. Due to its characteristic egg-shaped housing, the FRM in Garching has become a distinctive landmark. Forschungszentrum Jülich, at that time known as the “Kernforschungsanlage Jülich”, hosted two neutron sources. In subsequent decades, friendly competition between the two neutron science centres led to numerous innovations in neutron methods and technology. However, operations at every neutron source eventually come to a natural end and those at FRM were wound down in 2000 followed by those in Jülich in 2006. At this point, the time had come to join forces.

In 2004, Jülich and the Technical University of Munich (TUM) signed a cooperation agreement to operate neutron scattering instruments, previously housed in Jülich, at the new neutron source FRM II. In this way, the outstation of the Jülich Centre for Neutron Science (JCNS) was founded. A total of seven instruments were moved from Jülich to Garching to ensure the continuation of cutting-edge research with neutrons.

The next milestone was achieved at the end of 2010 by the signing of the cooperation contract between the TUM and the Helmholtz Centres in Jülich, Geesthacht, and Berlin. Based on a remarkable level of funding made available for research for the period 2011 – 2020, the instrument suite could be considerably increased and improved. These joint activities are embedded in the national and European neutron strategy.

Now the aspirations and endeavours of the MLZ have led to the next big step forward. The construction of two new buildings on the campus has already begun. The new laboratory and offices of Forschungszentrum Jülich and the science and technology building of the TUM have been designed to become a second landmark. With a total investment of around €30 million, the addition of 9,300 m² of floor space, including modern, well-equipped laboratories for the users and local scientists, will constitute a remarkable leap forward. It is expected that after their completion in 2019, the new buildings will make the MLZ even more attractive for the German and international neutron user community.



Prof. Dr. Sebastian M. Schmidt

*Member of the
Board of Directors of
Forschungszentrum Jülich*

Read more

**in our report about the cut of
the spade on p. 17!**

- 05 • Slow dancing with neutrons:
High resolution spectrometers at the MLZ

SPECIAL FEATURE

- 11 • First neutrons at KOMPASS
- 12 • New set-up for polarized neutron diffraction in magnetic field at POLI
- 14 • NICOS: Past, present and future
- 15 • Recent upgrades at the TOF reflectometer REFSANS

INSTRUMENTATION

- 16 • First Röntgen Ångström Cluster Winter School on Materials Science (MATRAC-2)
- 17 • New buildings for the Heinz Maier-Leibnitz Zentrum
- 18 • MLZ@DPG
- 18 • Three axes resolution workshop at MLZ
- 19 • DGK Workshop "Breaking the Walls"

EVENTS

- 20 • Development of a new fuel for FRM II
- 22 • ACCELERATING Europe's leading research infrastructures

SCIENCE & PROJECTS

- 23 • From Serpong to Garching: exchange and education
- 24 • Newly arrived
- 26 • The UCN group
- 28 • New brochure "Safety first"
- 29 • Call for proposals

INSIDE

- 30 • Six years as chair of the Komitee Forschung mit Neutronen

OUTSIDE

- 32 • Use of the MLZ beam time 2016
- 33 • MLZ proposal round 2017-I
- 34 • Upcoming
- 34 • Reactor cycles 2017

USER OFFICE

Slow dancing with the neutron:

High resolution spectrometers at the MLZ

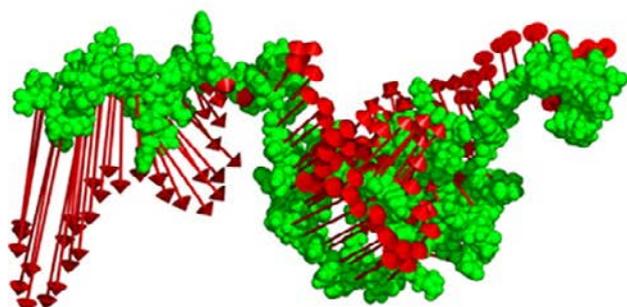
High energy resolution at atomic and mesoscopic length scales is provided by a suite of neutron spectrometers, each with its own strength and field of specialisation. The two most prominent fields of neutron scattering, magnetic structures and soft matter systems, are addressed with these instruments. The accessible energy transfer of the high resolution spectroscopy suit ranges from meV down to the neV range, covered by the techniques of time-of-flight spectroscopy by way of backscattering spectroscopy to neutron (resonance) spin echo spectroscopy. Part of the instruments measure the scattering function $S(q,\omega)$ as a function of scattering vector q (or the modulus of it) and the energy transfer $\hbar\omega$ during the scattering process. Time-of-flight spectroscopy uses a chopped neutron beam defining the arrival of the neutrons at the sample and measuring the travel time from the sample to the detector to achieve the sensitivity to the energy transfer during scattering. Backscattering also measures the scattering function $S(q,\omega)$, defining the incoming and outgoing energy by Bragg diffraction at crystals. The highest possible energy resolution is achieved in backscattering geometry, variation of the incoming energy is provided by a moving monochro-

mator crystal which introduces a Doppler shift to the neutron energy. The Fourier transform of the function $S(q,\omega)$ from energy into the time domain, i.e. the intermediate scattering function $S(q,t)$ is measured with neutron (resonance) spin echo spectroscopy. By using the neutron spin of each neutron as an individual stop watch the resolution can be increased since it does not depend any more on the wavelength spread $\delta\lambda/\lambda$ which results in an intensity penalty for increased resolution.

J-NSE

The J-NSE neutron spin echo spectrometer covers length- and time-scales relevant for thermal fluctuations and diffusion in soft matter systems. Examples are domain motion of proteins [j1,j2], diffusion in crowded environment [j3] or phospholipid membrane fluctuations [j4] under natural (physiologically relevant) conditions. But it is not strictly restricted to soft matter applications, also paramagnetic scattering such as nuclear spin waves or spin dynamics in spin glasses are possible applications of the classical NSE technique.

IDP Dynamics



Neutron Spin-Echo

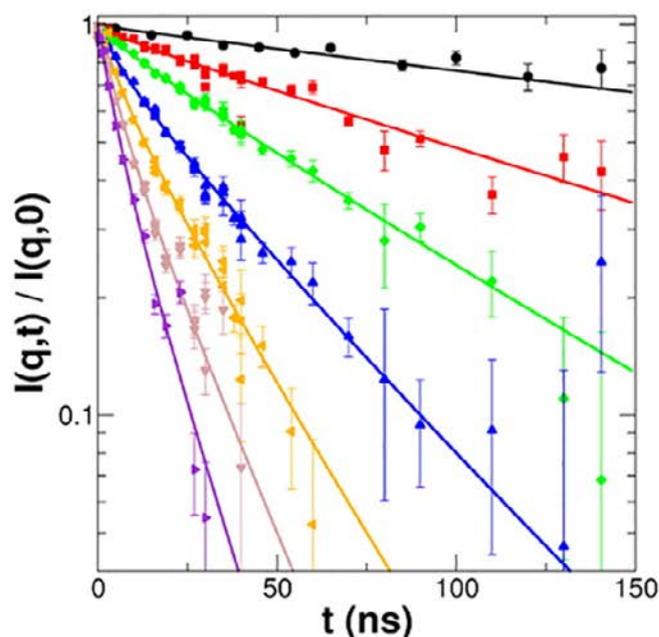


Fig. 1: Internal dynamics of the Intrinsically Disordered Myelin Basic Protein. Reprinted with permission from: A. M. Stadler, L. Stingaciu, A. Radulescu, O. Holderer, M. Monkenbusch, R. Biehl, D. Richter; J. Am. Chem. Soc. 2014, 136, 6987-6994. DOI: 10.1021/ja502343b. Copyright © 2014 American Chemical Society.



Fig. 2: Empty carriers, after the main coils have been removed, waiting for the cool superconducting solenoids.

As an example of a J-NSE application, fig. 1 shows results of the Intrinsically Disordered Myelin Basic Protein, which showed that the protein undergoes mainly fluctuations along the red arrows in the left part of the figure, and is, although structurally like as Gaussian chain similar to a polymer chain in solution, not following the characteristic Zimm dynamics [j1].

Currently, a large upgrade is on the way for a significant increase in resolution [j5]. The heart of the instrument, the two main solenoids which provide homogeneous magnetic fields with a very high accuracy, are being replaced with new coils of an innovative design. The copper coils consuming up to 160 kW of electrical power are replaced by superconducting coils (with a much smaller peak power). Instead of a single main coil a set of five pairs of fully compensated coils is assembled in a way that reduces the intrinsic inhomogeneity of the magnetic field integral (directly proportional to the achievable Fourier time).

RESEDA

The resonance spin echo spectrometer for diverse applications RESEDA is the first of its kind – a longitudinal neutron resonance spin echo spectrometer (INRSE) [r1]. It can be seen as a hybrid between a classical NSE spectrometer with longitudinal geometry and a conventional transverse NRSE instrument. Thus advantages of both techniques can be exploited, namely lower and shorter magnetic fields of NRSE in comparison to conventional NSE while keeping the possibility to use well established NSE correction elements such as Fresnel coils. Furthermore, due to the resonant spin flip in the middle of the static magnetic field, the method is self-correcting, leading to significant lower field inhomogeneities.



Fig. 3: Secondary spectrometer arms of RESEDA, NRSE arm with black detector box, MIEZE arm with CASCADE detector in the blue shielding box.

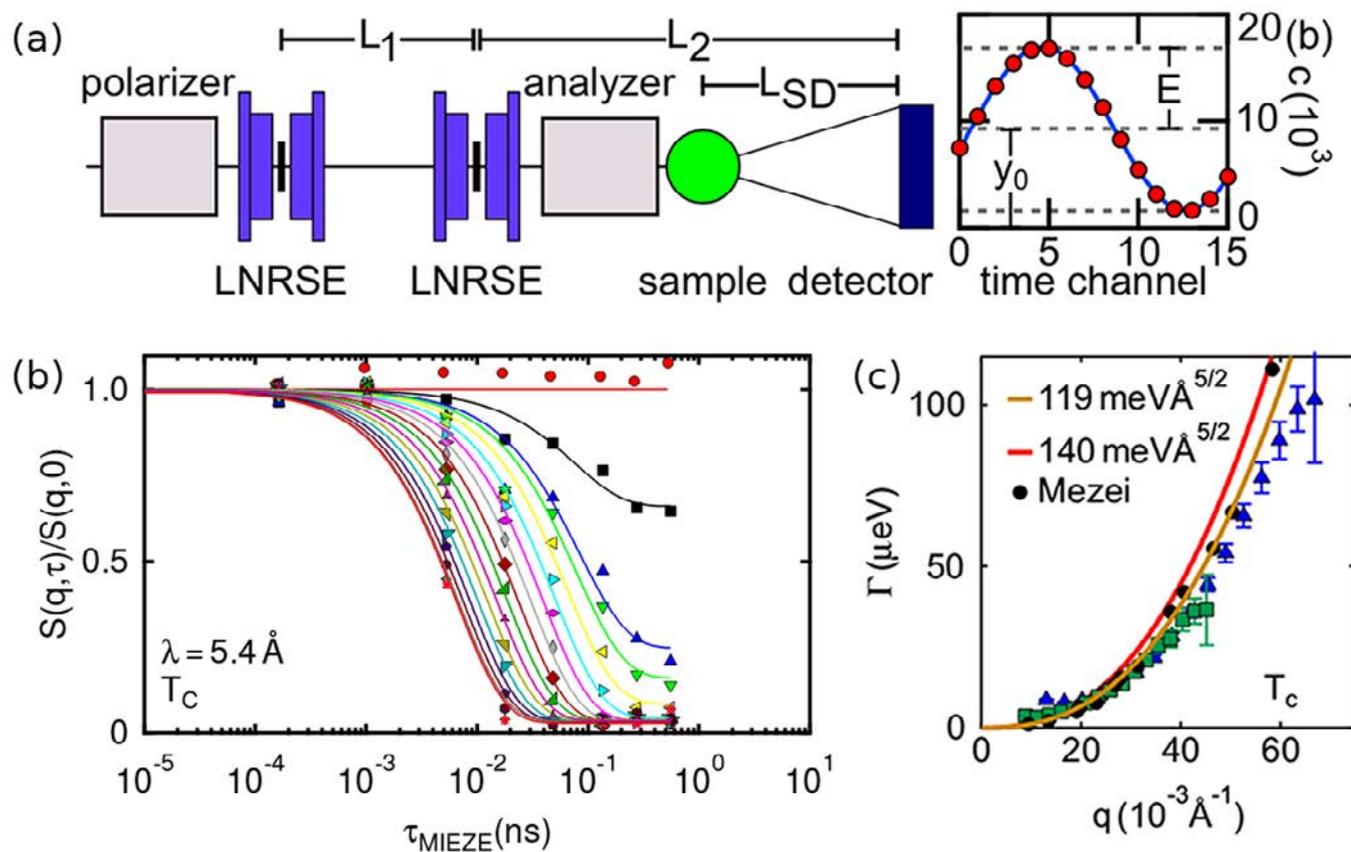


Fig. 4: (a) MIEZE set-up; (b) Critical fluctuations at the Curie point of iron for $q=0.013\text{\AA}^{-1}$ (red stars) to 0.068\AA^{-1} (black squares) studied by MIEZE; (c) q -dependent linewidth

Typical applications of NRSE cover dynamics ranging from tens of ps to tens of ns in structures from atomic to molecular length scales. Most prominent fields of investigations are polymer (self)-diffusion, protein folding and water dynamics in clays [r2].

For samples with strong incoherent scattering, i.e. rich hydrogen content, magnetic moment or under depolarizing conditions such as large magnetic fields the MIEZE (**m**odulation of **i**ntensity with **z**ero **e**ffort) technique offers access on similar time scales. Here the

information of the scattering event is encoded in the intensity modulation of the neutron beam instead of the Larmor phase (c.f. fig 4(a)). RESEDA is the worldwide only instrument employing this method routinely. It offers a large dynamic range of 6 orders of magnitude in spin echo time and is used - but not limited to the fields of quantum phase transitions, spin glasses and superconductivity as well as skyrmion physics. As an example, the q -dependence of critical fluctuations at the Curie point of iron have been studied, underlining the importance of dipolar interactions [r3].

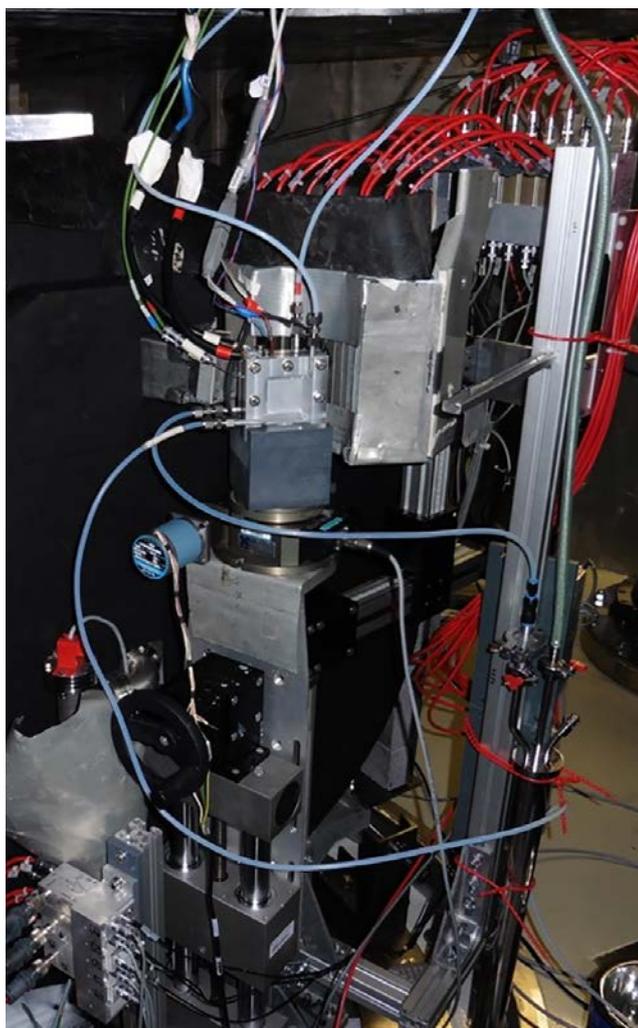


Fig. 5: Fuel cell set-up in operando installed at SPHERES [s3].

SPHERES

The neutron backscattering spectrometer SPHERES (**SP**ectrometer for **H**igh **E**nergy **RES**olution) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It covers a dynamic range of $\pm 31 \mu\text{eV}$ with a high energy resolution of about $0.66 \mu\text{eV}$ and a good signal-to-noise ratio. The intensity has been recently doubled by the upgrade of the PST chopper. Further improvement of the instrument performance is expected from the planned upgrade of the focussing guide and the introduction of a background chopper.

The spectrometer enables investigations on a broad range of scientific topics- from the classical applications of backscattering like hyperfine splitting or rotational tunneling [s1] to investigations on new materials like protein-polymer hybrids [s2] or high temperature polymer electrolyte fuel cells [s3]. It is suitable to study the dynamics in soft matter materials like polymers [s4] or proteins [s5] or observe the motion of water in confined geometry [s6] or hydrogen diffusion in various system. In fig. 6 an example of a SPHERES application is shown, where the mobility of water on the surface of tau proteins and its fibers were investigated [s7], in order to better understand the mechanisms of fiber formation, which also occurs in neurodegenerative diseases.

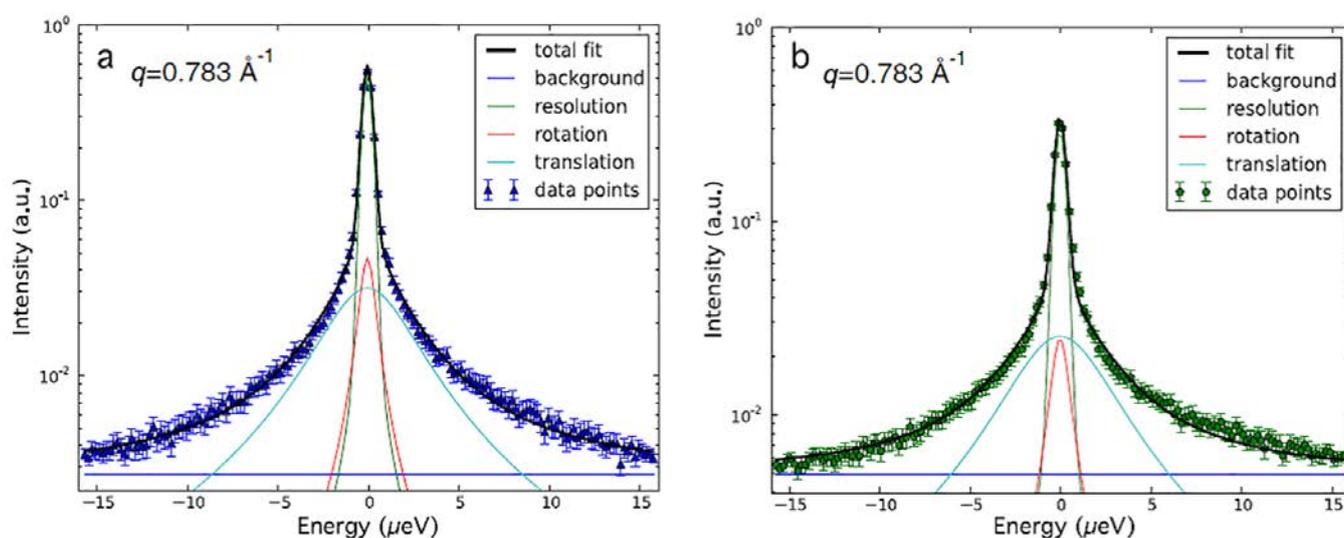


Fig. 6: QENS spectra of (a) D-fiber- H_2O and (b) D-tau- H_2O . Reprinted from Y. Fichou et al., PNAS 112, 6365 (2015) [s7].

The standard sample environment, a cryofurnace, covers a temperature range of 3-650 K, which can be extended to the 100 mK range by a dilution insert. A new furnace allows to access temperatures up to 1800 K. Usually it is also possible to accommodate user provided equipment like pressure cells or even a fuel cell set-up in operando (see fig. 5, [s3]).

TOFTOF

The direct time-of-flight spectrometer TOFTOF (see fig. 7) is optimised for the investigation of the dynamics in disordered materials on time-scales of picoseconds and length scales of Ångströms. The energy resolution at the elastic peak can be freely tuned between 3 meV and 2 μeV thus bridging the gap between thermal spectrometers on the one side and backscattering technique on the other side.



Fig. 7: The instrument TOFTOF in the Neutron Guide Hall West.

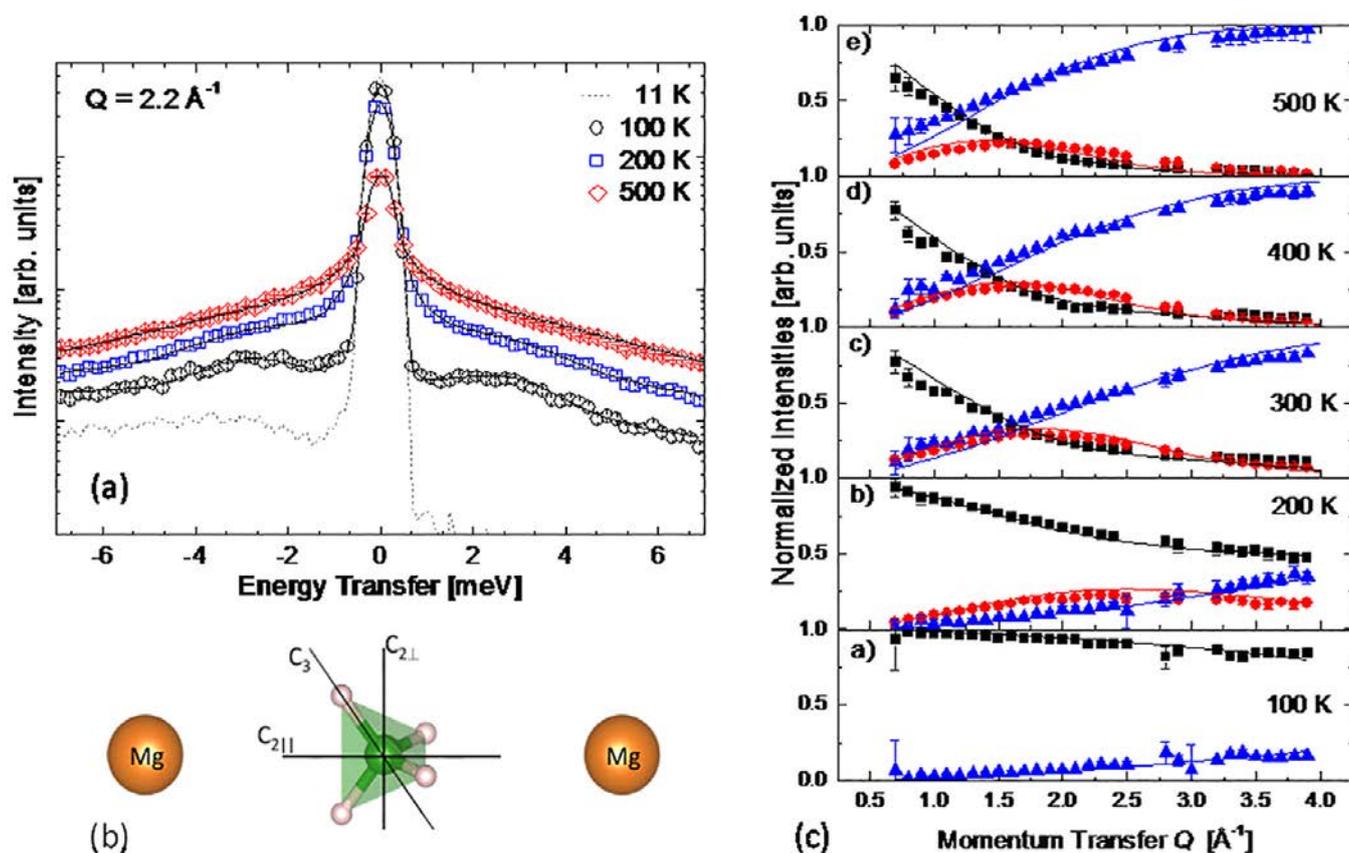


Fig. 8: Quasielastic scattering of $\beta\text{-Mg}(\text{BH}_4)_2$ at different temperatures: (a) The combined analysis of the Elastic and Inelastic Incoherent Structure Factors (see (c), EISF (black symbols) and QISFs (red, blue symbols)) was used to disentangle the localised motions of the BH_4 -tetrahedra in the material. A schematic representation of the local structure is shown in (b).

The scientific questions addressed encompass a broad range of fields such as quantum phenomena, materials science such as the diffusion in metal melts [t1], hydration water in thermosensitive polymers at the phase transition [t2] in soft matter research, or the lipid mobility in the presence of the peptide amyloid-beta relevant for Alzheimer's disease [t3] research.

Fig. 8 shows data measured at TOFTOF on the complex hydride beta-Mg(BH₄)₂ [t4], a material that is of interest for solid state hydrogen storage due to its high gravimetric hydrogen content. Measurements at two different energy resolutions were used to disentangle the contributions of localised rotations and low lying vibrations, which play a crucial role in the stability of the phase and most likely drive the phase transition from the alpha- to the beta polymorph.

Recent upgrades of TOFTOF include the installation of a focusing guide section as the last section of the guide which can be chosen as small beam spot alternative to the linear tapered guide, the possibility to fit the HTS magnet (with the vertical field direction) offering a magnetic field of up to 2.2T and the implementation of data reduction routines in the Mantid framework for quick and easy-to-use data inspection capabilities during the experiments.

*O. Holderer, M. Zamponi (JCNS);
C. Franz, W. Lohstroh, O. Soltwedel (FRM II)*

References

J-NSE

- [j1] Stadler A.M. et al, JACS 136, 6987 (2014)
- [j2] Stingaciu L. R. et al, Sci. Rep. 6, 22148 (2016)
- [j3] Bucciarelli S., et al, Science Advances, 2, e1601432 (2016)
- [j4] Jaksch S., et al., submitted
- [j5] Pasini S. et al, Meas. Sci Technol. 26, 035501 (2015)

RESEDA

- [r1] Krautloher M. et al, Rev. Sci. Instr. 12 125110 (2016)
- [r2] Marry V., et al, J. Phys. Chem. C 117, 15106 (2013)
- [r3] Kindervater J. et al. Phys. Rev. B 95, 014429 (2017)

SPHERES

- [s1] G. Bator et al., Chem. Phys. 459, 148 (2015)
- [s2] F.-X. Gallat, J. Am. Chem. Soc. 134, 13168 (2012)
- [s3] Khanefit M., et al., AIP Conference Proceedings, accepted
- [s4] D. Bhowmik et al., Macromolecules 47, 304 (2014)
- [s5] M. Monkenbusch et al., J. Chem. Phys 143, 075101 (2015)
- [s6] A. Soininen, J. Chem. Phys. 145, 234503 (2016)
- [s7] Y. Fichou et al., PNAS 112, 6365 (2015)

TOFTOF

- [t1] Z. Evenson et al., Appl. Phys. Lett. 108, 121902 (2016)
- [t2] M. Philip et al., J. Phys. Chem. B 118, 4253 (2014)
- [t3] M.A. Barrett et al., Soft Matter 12, 1444 (2016)
- [t4] L. Silvi et al., Phys. Chem. Chem. Phys. 18, 14323 (2016)



Scan the qr-code and find all information about spectroscopy on our web page!

First neutrons at KOMPASS

KOMPASS is the newest, polarized cold neutron three axes spectrometer (TAS) undergoing its final construction phase at the MLZ. In contrast to our other TASs, KOMPASS is equipped with a unique permanently installed parabolically focussing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam with expected polarization above 98%. The exchangeable front-end part of the guide system allows adapting the energy- and momentum-resolution of the instrument for a particular experiment. Highest flux, high energy- and reduced momentum-resolution are obtained in the configuration with a parabolic front-end section, whereas the straight section in combination with an optional collimation is the optimal choice for measurements when a high transverse momentum-resolution is required.

Variation of the incident neutron energy within the range from $2 \leq E \leq 25$ meV is realised via tuning of the take-off angles of the adjustable doubly-curved monochromator array consisting of 19×13 highly oriented pyrolytic graphite (HOPG(002)) crystals. The bottom panel of the figure shows two neutron beam images as obtained when neutrons were extracted for the first time. The shielding of the neutron optical components, of the velocity selector, and of the monochromator turned out to be well adapted and the mechanics of the neutron optics and that of the monochromator worked as expected.

Currently we are working on assembling the sample table and the detector/ analyzer tower. The scattered neutrons will be analyzed by a doubly-focussing array of 21×11 HOPG(002) crystals. Spin-polarization analysis will be performed by a trapezoidal single V-cavity consisting of 13 channels. The expected polarization efficiency of this device exceeds 96% for neutron energies $E_f < 15$ meV. Finally, the neutrons will be registered by a standard position sensitive ^3He -counting tube.

At the same time the preparation and development of the sample environment is proceeding. For controlling the neutron polarization either a 3rd generation ILL CryoPAD or a set of Helmholtz coils will be available at the first stage; later also a mini MuPAD will be in-

stalled. The optimisation of the neutron polarization throughout the spectrometer will provide a very competitive three axes spectrometer for the investigation of weak magnetic order, complex magnetic structures (e.g. multiferroics), quantum magnets, quantum critical fluctuations, systems of reduced dimensions (e.g. thin films and multi-layer structures), as well as for experiments under extreme conditions.

In the light of the recent progress in the construction of KOMPASS and with the support of the technical staff of FRM II we are confident that the beamline will produce first scientific results already in 2017.

The construction of KOMPASS is funded by the BMBF through the Verbundforschungsprojekt 05K16PK1.

*D. Gorkov (Universität zu Köln), G. Waldherr (TUM),
M. Braden (Universität zu Köln), P. Böni (TUM)*



Upper panel: photo of the beamline KOMPASS. Bottom panel: Images as acquired using a neutron camera for the monochromator in the flat (left) and doubly focussing configuration (right).

New set-up for polarized neutron diffraction in magnetic field at POLI

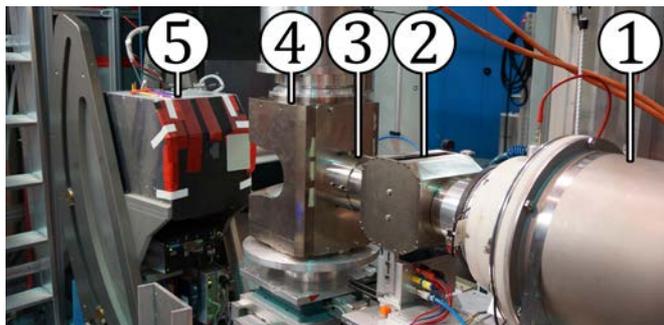


Fig. 1a: Set-up option for flipping ratio measurements with 1) Polarizer SFC in μ -metal shield, 2) Mezei spin flipper in iron shield, 3) shielded guide field, 4) HTS magnet and 5) lifting counter.

The **Polarisation Investigator (POLI)**, operated by RWTH Aachen in cooperation with JCNS at MLZ, is dedicated to the investigation of complex magnetic structures of single crystals and their behavior under varying external conditions like temperature, pressure and magnetic or electric fields.

The instrument, positioned in front of the hot source, uses short wavelength neutrons, provided by either a double focusing Cu (220) or a vertically focusing and horizontally bent Si (311) monochromator. The available wavelength bandwidth is between 0.55 Å and 1.15 Å, reaching from hot to thermal neutrons.

In addition to the available spherical neutron polarimetry in the zero field [1], the instrument POLI was recently extended with a set-up for polarized neutron diffraction in a magnetic field. It uses the new high temperature superconducting magnet with a maximum field of $B_{\max} = 2.2$ T, manufactured by HTS 110 New Zealand.

Due to the large openings of the HTS magnet, giving 130° horizontal and 40° vertical access to the scattered beam, the set-up can be operated in two different options: It can either be used with a lifting counter for out of plane flipping ratio measurements (fig. 1a) or with the polarization analyzer for uniaxial polarization analysis (fig. 1b). Moreover, the wide openings and the large sample area allow to insert a cryostat for sample temperatures between 90 mK and 500 K or the usage of a pressure cell in the magnetic field.

The beam polarization and analysis is achieved on POLI by using optimised ^3He spin-filter cells (SFC). In

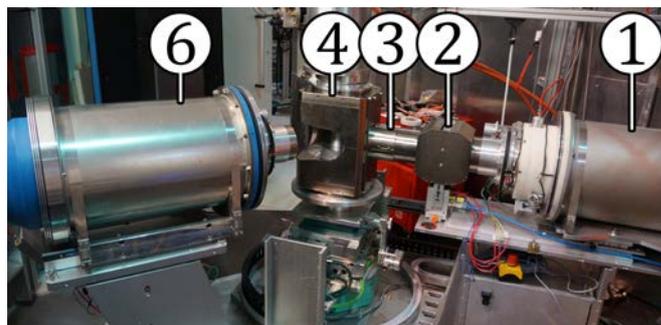


Fig. 1b: Set-up option for uniaxial polarisation analysis with 6) Decpol (analyzing SFC in μ -metal shield and detector).

general, the combination of high magnetic fields with ^3He SFCs is seen as difficult, since the stray fields of the magnet can disturb the polarization of Helium gas in the cells [2]. But for the HTS magnet, due to its iron yoke the stray fields are rather low (5 mT at a distance of 1.8 m). Thus, the μ -metal shielding surrounding the SFCs magnetostatic cavity effectively screens the stray field and no polarization losses were observed up to highest available field in spite of the short distance between polarizer and magnet (fig. 2).

HTS magnet has a symmetric field geometry and thus, the transition point between the main and fringe field lies in the neutrons' way. To avoid the depolarization of the neutrons on this zero-field region, a dedicated guide field was developed to connect the field in the polarizer to the main field in the magnet without disturbing the neutron polarization. The guide consists of two main parts. The first one is a Mezei flipper optimised for the hot neutrons, shielded from the stray field of the magnet by an thick iron box, and placed into homogeneous guide field of around 30 G, produced by permanent magnets. This part is located directly after the polarizer (pos. 2 in fig. 1). The second one is the connection between the flipper and HTS magnet. It consists of two iron poles going inside the magnet and guiding its main field toward the flipper to suppress the zero point. These flat poles are shielded by an iron cylinder and directly mounted to the magnet yoke (pos. 3 in fig. 1).

The individual parts of the guide field and the flipper were optimised by finite element simulations using COMSOL Multiphysics® software as part of the bachelor thesis of Henrik Thoma.

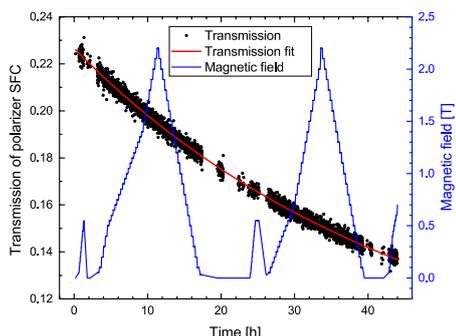


Fig. 2: ^3He SFC transmission and field in HTS magnet over time for an arbitrary experiment. There is no influence of the magnetic field on the cell relaxation time of $T_1 = 127$ h.

To characterise the polarization feed-through of the new set-up using half-polarized set-up option 1 (fig. 1a), an analyzing Heusler (Cu_2MnAl) single crystal was placed in the magnet. The (111) reflection of analyzers was measured as function of the applied magnetic field. From this data, the polarization feed-through of the set-up was calculated assuming the analyzing efficiency of saturated Heusler crystal for short wavelength to be about 0.95. The results shown in fig. 3, denote a value of one corresponding to no polarization losses and zero to a complete depolarization. One observes the almost perfect polarization feed-through at the fields above 1 T. Since the Heusler crystal is not fully magnetised for small magnetic fields, it loses its analyzing power and the calculated polarization feed-through breaks down below a certain field. To cover this field range, a nuclear reflection of hematite ($\alpha\text{-Fe}_2\text{O}_3$) crystal was measured with set-up option 2 (uniaxial polarization analysis), where a second ^3He SFC serves as analyzer. The results are shown with red symbols in fig. 3. In conclusion, a high polarization feed-through of 98.5% over the complete field range of the HTS magnet was verified.

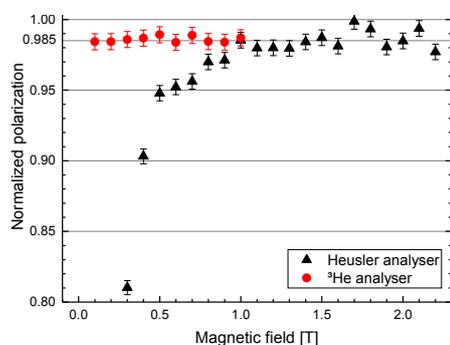
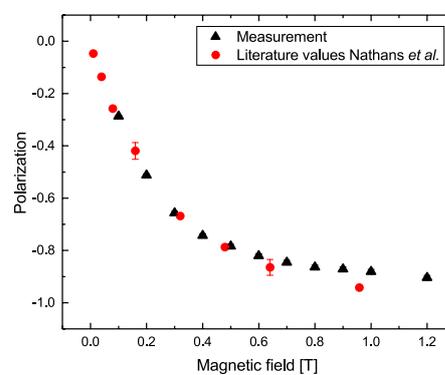


Fig. 3: Polarization feed-through of the setup measured with option a) and a Heusler single crystal as analyzer and option b) with ^3He SFC as analyzer.

As first measurement with new set-up the antiferromagnetic domain movement at room temperature in hematite crystal was studied. Since hematite possess-

es a rhombohedral structure with space group $R\bar{3}c$, trigonal domains are formed in the hexagonal basal plane above the Morin temperature $T_M = 259$ K. Without external magnetic field, the domains are equally distributed. Applying a magnetic field along a certain direction, favours domains with antiferromagnetic spins perpendicular to the field. Thus, the domain distribution changes. If the field is high enough, a saturated mono-domain state can be reached. To study the antiferromagnetic domain population as function of applied field we choose the set-up option 2 which allows the polarization analysis along field direction. For

Fig. 4: Comparison between POLI measurements using new setup and literature data regarding single domain formation in $\alpha\text{-Fe}_2\text{O}_3$ as function of applied magnetic field at room temperature.



the purely magnetic Bragg reflection (003) and hexagonal axes of the crystal oriented in the scattering plane and magnetic field normal to the scattering plane the presence of the different domains will depolarize the beam. Measuring spin-flip and non-spin-flip contributions separately, it is possible to determine the polarization grade of the scattered beam as function of the applied field and conclude about the domain population. The measured final polarization, which is related to the domain distribution, is shown in fig. 4. It shows that field of about 0.7 T needs to be applied to create a quasi-mono-domain state in antiferromagnetic hematite ($\alpha\text{-Fe}_2\text{O}_3$). Our result is in a very good agreement with the literature values from Nathans et al. [3] demonstrating the high accuracy of the new set-up. Polarized diffraction experiments in magnetic field are available now for the users on POLI.

V. Hutanu, H. Thoma
(RWTH Aachen)

References

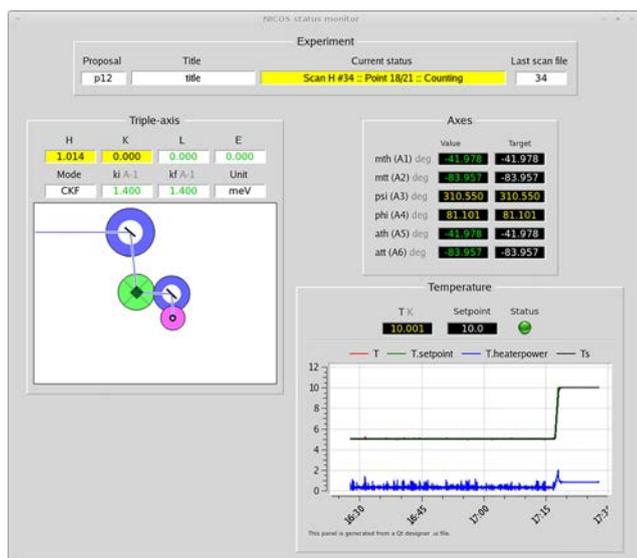
- [1] V. Hutanu, J. Large-Scale Res. Facil. 1, A16 (2015)
- [2] J. Dreyer, L.-P. Regnault, et al., Nucl. Instr. Meth. Phys. Res. A 449 638 (2000)
- [3] R. Nathans, P. J. Brown et al., Phys. Rev. 136 (6A), A1641 (1964)

NICOS: Past, present and future

The start of cycle 42 saw KWS-3, MARIA as well as SPODI starting user experiments with NICOS, the MLZ-wide standard instrument control software. This brings the number of instruments running on NICOS to over twenty, with only a handful still to do. Together with the NICOS changeover, most instruments also have seen an extensive overhaul to low-level components: old hardware was replaced, PLC systems were updated and brought to a standard interface, and the device server software was switched from TACO to Tango.

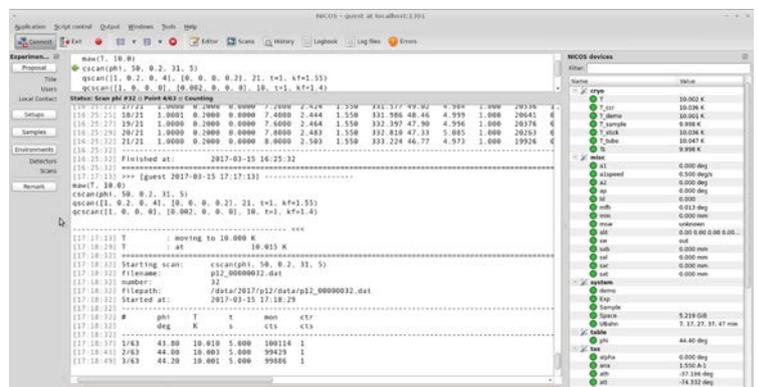
Since its conception in 2008, the current version of NICOS has been in continuous development driven by the experience of the instrument scientists. Rooted in an earlier incarnation that was conceived in the beginning days of the FRM II, it aims to provide users and local scientists alike with a modern, flexible, and intuitive way to direct their experiments. In particular, the decision to use Python as a scripting language has proven invaluable, as it has become one of the most widely used tools in scientific computing.

Using a code review system and modern best practices of code development, the same code base can now be used on all instruments and the various services NICOS provides are acknowledged by instrument scientists and users.



NICOS status monitor in an exemplary TAS configuration.

In 2012, MLZ decided to use NICOS as the standard control system for all instruments, at which point it became a joint MLZ effort to fill the needs of very different classes of instruments. For each, the NICOS core is extended with custom components that help with the idiosyncrasies of the particular method, ranging from a quick way to schedule measurement of lots of samples in numerous configurations at SANS instruments to the extreme flexibility required at test beamlines. A unified way of handling optional components, especially sample environment, with self-contained control boxes makes sharing them between instruments quick and painless.



NICOS GUI connected to a demonstration session.

Currently the basic task of migrating instruments to NICOS is progressing at a steady pace, allowing us to tackle more of the advanced features such as integrating NICOS with the new proposal system GhOST, helping users stay abreast of the increasing volumes of data collected, and more tightly connecting instrument control and data evaluation. The latter is simplified by the increasing international momentum towards common frameworks for data treatment, supported by our Scientific Computing Group. Furthermore, starting in 2015 we formed collaborations with the instrument control groups at ESS and ISIS, both of which have expressed interest in NICOS and the possibility of using it at least parts at their facilities.

Finally, since instrument control serves the user, we depend on your input! Please don't hesitate to let your local contact know of any problems, annoyances or suggestions concerning NICOS: we are happy to help improve your experience.

G. Brandl (JCNIS), E. Faulhaber (FRM II)

Recent upgrades at the TOF reflectometer REFSANS

REFSANS is the time-of-flight (TOF) reflectometer with **G**razing **I**ncidence **S**mall **A**ngle **N**eutron **S**cattering (GISANS) option operated by GEMS at MLZ. The instrument was designed to study the structure of liquid/air interfaces (fig. 1). These systems make it mandatory to use a horizontal configuration which is best achieved via the TOF operation. A complex collimation setup is then necessary in order to bend the beam to selected incident angles onto the sample while controlling the divergence both vertically and horizontally. During the last years the beamline attracted experiments to also investigate solid samples. In these cases the TOF mode of operation was exploited to perform GISANS measurements but also help to setup in-situ measurements (sputtering chamber, high pressure cells, liquid cells...) as well as study kinetics. In those cases where a high time resolution is needed, using the TOF mode allows to collect the full scattering pattern in one shot and repeat this acquisition many times in order to improve statistics. A monochromatic instrument would in this case have to perform a time consuming angular scan. Most of these experiments are performed on samples smaller than the typical Langmuir trough used for liquids and a continuous instrument upgrade program has been pursued with that in mind.

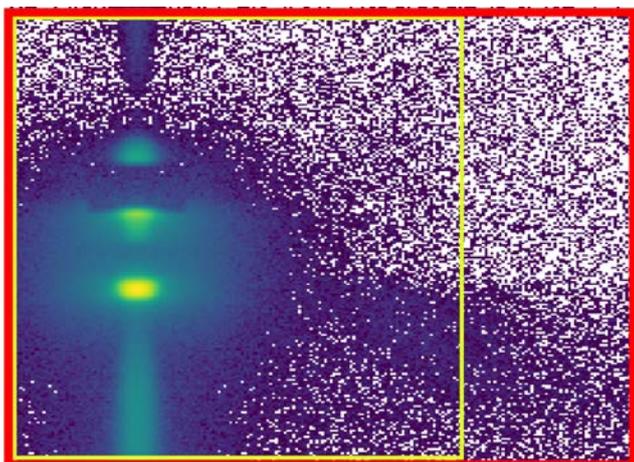


Fig. 1: Reflectivity of the D_2O /air interface (measured in 45 min), the inset shows the Langmuir trough installed on the goniometer.

A slower chopper for faster kinetics!

The frame overlap chopper has received new disks featuring two symmetric windows. Using this simple trick it is possible to get twice as many pulses from the chopper without changing its rotation speed and hence keeping the motor and transmission design more reliable. Together with recent improvements

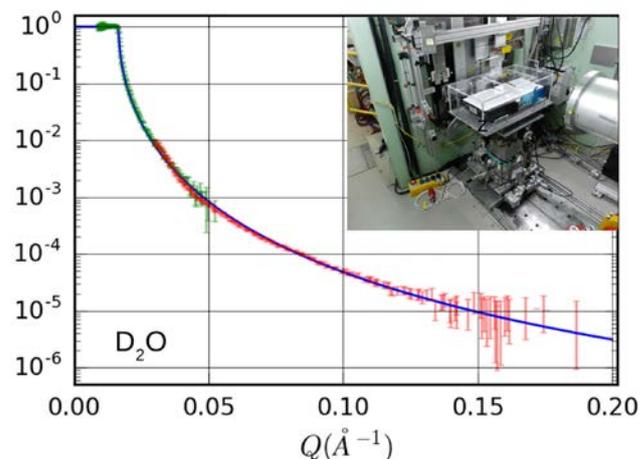


Fig. 2: The old detector (yellow line) would have cut a Bragg peak making it necessary to measure at two positions. The new detector (red line) catches the full pattern.

in the data acquisition set-up which allow to keep the detector constantly under illumination, this benefits greatly the kinetics experiments which are becoming increasingly requested.

Eyes wider open!

The detector width has been increased by 40%, (surface is now $680 \times 500 \text{ mm}^2$). The new ^3He multiwire chamber with a pixel size of 2.5 mm makes it possible to record patterns over a wider Q range in less time (fig. 2). For specular reflectometry, the increased width also leads to an overall intensity increase of about 30% since it is now possible to accept more horizontal divergence of the primary beam.

No longer let neutrons fall!

In early May, a new high resolution slit system has been positioned very close to the sample in order to control at best the beam footprint on smaller surfaces and reduce the importance of the gravity induced beam drop. This makes it possible to use wider slits settings for smaller samples. The intensity gain is up to a factor two for typical measurements.

You said «Polarization»?

A double V broadband polarizing cavity (Swiss Neutronics) was installed together with a in-collimation spin-flipper. This set-up offers the option to polarize the full beam size ($170 \times 12 \text{ mm}^2$). It will benefit projects involving for instance magnetic nanoparticles as well as it will enable to use polarization analysis to suppress the incoherent background which is especially harmful to soft-matter systems studies.

J.-F. Moulin (HZG)

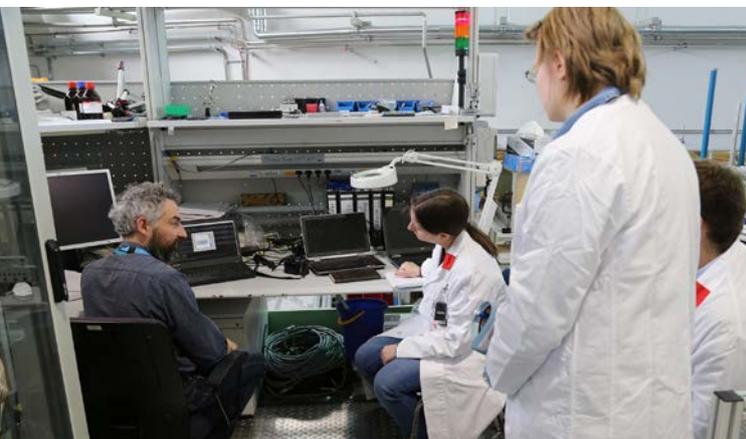
First Röntgen Ångström Cluster (RAC) Winter School on Materials Science (MATRAC-2)



© P. Baur (TUM)

44 students and young scientists from Germany, Sweden, and ten other countries met in the week around carnival (Feb. 26th – March 03rd) in Utting at the beautiful Ammersee.

The lectures given by sixteen experts from Swedish and German universities as well as research centres and from the MLZ ranged from the fundamentals of elastic and inelastic scattering of neutrons and X-rays over details of experimental techniques to modern functional materials and biomaterials. The school thus provided a systematic overview on the application of neutrons and synchrotron radiation for the structural and dynamical analysis of materials and focussed on neutron scattering and imaging experiments.



© P. Baur (TUM)

Experiment at REFSANS.

This focus was further enhanced by a two-day practical course with “hands-on” experiments at MLZ instruments in Garching. Every participant got to know four different instruments. In the final feedback session of the school this was highly appreciated, and the dedication of the MLZ instruments scientists was mentioned many times.

The fairly remote school location outside the vil-

lage of Utting fostered many scientific discussions at the poster sessions (where most of the participants presented their work) and also after dinner. One of the dinners was actually taken just below the old monastery of Andechs with many samples of local specialties.



© M. Müller (HZG)

A (seminar) room with a view.

The school was funded by Sweden and Germany (Federal Ministry for Education and Research / BMBF and the Northern German federal states) and by the European Union (SINE2020) and organised by Helmholtz-Zentrum Geesthacht together with the MLZ and a RAC programme committee.

M. Müller (HZG)

New buildings for the Heinz Maier-Leibnitz Zentrum

© U. Benz (TUM)



“The research neutron source has an exceptional worldwide reputation,” said Stefan Müller, Parliamentary State Secretary at the German Federal Ministry for Education and Research. *“A fundamental question of research policy is to what degree we are able to attract the best minds for research. To this end, we need an optimal framework, a creative environment and infrastructures, in other words, equipment and modern buildings like the ones being built here in Garching. They form a cornerstone in further improving the attractiveness of Germany as a base of science.”*

The number of scientific instruments at the Garching research neutron source has grown in recent years to 27, with six further instruments currently under construction. Since the new instruments require additional operators, the size of staff continues to grow. Two new buildings will alleviate the acute shortage of space and celebrated their ground-breaking on February 20th.

Over 400 people work at FRM II and the Heinz Maier-Leibnitz Zentrum (MLZ), on top of this come some 1000 guest scientists who also need space for experiments and offices. As of 2019, the two new buildings will take shape in front of the “Atomic Egg”. The architectural office HENN conceived the design for the two facing, four-story buildings, which frame the view to the listed “Atomic Egg” erected in 1957.

The northern building was commissioned by the Bavarian government for the Technical University of Munich. The approximately 2000 m² of usable floor space will house a two-story workshop hall and offices. The southern building was commissioned by the German Federal Ministry of Education and Research. It will house 2550 m² of office and laboratory space for scientists of the Jülich Centre for Neutron Science (JCNS) and the Helmholtz-Zentrum Geesthacht. Overall construction costs have been slated at around €32 million.

“Today’s ground breaking for the new buildings of the Heinz Maier-Leibnitz Zentrum is a clearly visible signal for leading research with neutrons in Germany and Europe,” said the Bavarian Science Minister Ludwig Spaenle. *“The MLZ assumes a pioneering role in the collaboration of scientists from university and non-university research institutions.”*

“The new science buildings of the Heinz Maier-Leibnitz Zentrum will bring together which belongs together: people to people and laboratories to workshops,” said Thomas Brückel, director at JCNS and speaker of the MLZ management. *“New ideas and collaborations will be born over friendly cups of coffee. The new laboratories will enhance the powerful tool of research with neutrons and allow science at the MLZ to achieve further insights.”*

C. Kortenbruck, A. Voit (FRM II)



© W. Schürmann (TUM)

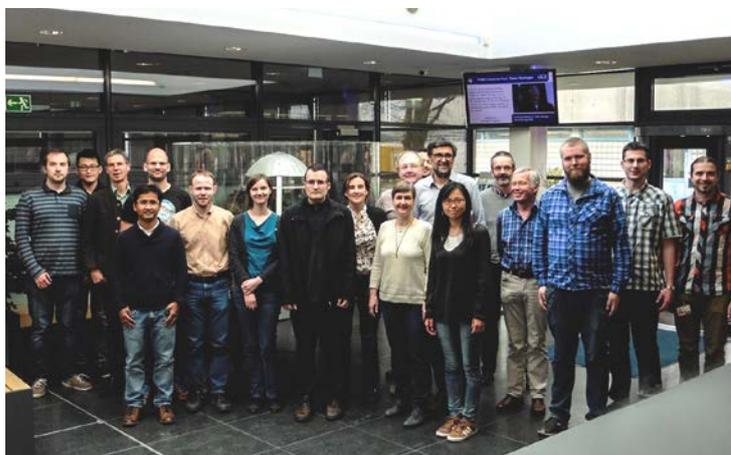
Camping at Dresden: The MLZ booth at the DPG Spring Meeting

For the first time, the MLZ booth was located in one of the tents at the DPG Spring Meeting of the Condensed Matter Section between March 19th and 24th. Weather at Dresden was still a little bit chilly, but we could welcome a lot of interested scientists among the 5914 participants. More of 1000 of them came from outside Germany – from neighbouring countries like Austria and Switzerland but also from France, the Netherlands, United Kingdom, many from the USA, Czech Republic, Sweden, Italy and Denmark. Even from Nepal, Island, Chile, and Qatar! All of them enjoyed the lively discussions in front of 1689 posters (us, too, because there were poster sessions in our tent each afternoon) in case they were not at one of the 5213 talks.

I. Lommatzsch (FRM II)



Three axes resolution workshop at MLZ Garching



On April 03rd and 04th, 2017 the quantum phenomena group of the MLZ organised a two-day workshop on software for calculating the resolution function of a three axes spectrometer and convoluting the data with theoretical models.

In the morning of the first day, an interesting overview talk of the different approaches to the three axes resolution was given by T. Weber (FRM II). J. Kulda (ILL) gave a very lively talk on his experience how to avoid problems in misinterpretation of resolution effects as real signals using these methods. G. Eckold (Univ. Göttingen) presented his approach to the determi-

nation of the resolution function and their use in disentangling signals in measurements using multiplexing analyzers. In the afternoon, T. Weber and J. Kulda presented their software packages for calculating the resolution – TAKIN and RESTRAX, respectively. P. Cermak (JCNS) gave also a short introduction into Ufit, a versatile fitting program for TAS data from most neutron centres developed by G. Brandl (JCNS). During the breaks and the lunch, which took place in the foyer of the lecture room the participants had time for longer discussions and exchanging experience with the software packages.

The morning of the second day was devoted to hands-on with examples using the different software packages. This gave the participants the possibility to explore the full extent of the software on real data. P. Cermak presented his view on good practice in TAS measurements and A. Schneidewind (JCNS) showed the different approaches how to detect and avoid spurious signals. In the late afternoon, a very lively discussion about the future needs of software for TAS measurements and how to publish the data together with the results took place.

R. Georgii (FRM II); P. Cermak, A. Schneidewind (JCNS)

DGK Workshop “Breaking the Walls: Complementary of Synchrotron and Neutron Scattering”

On March 30th and 31st, 2017, immediately after the annual meeting of the German Society of Crystallography (DGK) in Karlsruhe, a workshop took place dealing with the topic “Breaking the Walls: Complementary of Synchrotron and Neutron Scattering”. The workshop was organised by the DGK workgroup “Neutron Scattering” (speaker M. Meven) with support from colleagues from KIT (H. Ehrenberg, F. Weber) and JCNS (A. Schneidewind). Focussing on young scientists, the goal of the workshop was to present the peculiarities of the different kinds of radiation in order to show how to combine them in a smart way to get the most coherent and unambiguous answers to nowadays scientific topics. Aside from this, practical aspects were tackled like “How do I get beam time at a large scale facility as a user?”.

On Thursday afternoon, K. Röwer (HZB) and M. Meven (RWTH Aachen/ JCNS) presented the basics of synchrotron and neutron scattering as well as an overview of the corresponding facilities in two talks. On Friday morning, four talks were given by S. Rosenkranz (Argonne, USA), T. Schrader (JCNS), F. Weber/ F. Tissault (KIT) and M. Behrens (Universität Duisburg-Essen) about different topics related to fundamental and material sciences, each followed by lively discussions with the participants.

The strong wish of young scientists to get informed about state-of-the art methods outside their own laboratories for studies on nowadays scientific topics is visible also in the huge amount of more than fifty applications to the workshop. About one half of the participants also took the opportunity to use a guided tour of ANKA, the synchrotron source at Karlsruhe: They got a detailed insight into structure and organisation of a large scale facility on Friday afternoon.

M. Meven (RWTH Aachen/ JCNS)



© H. Ehrenberg (KIT)

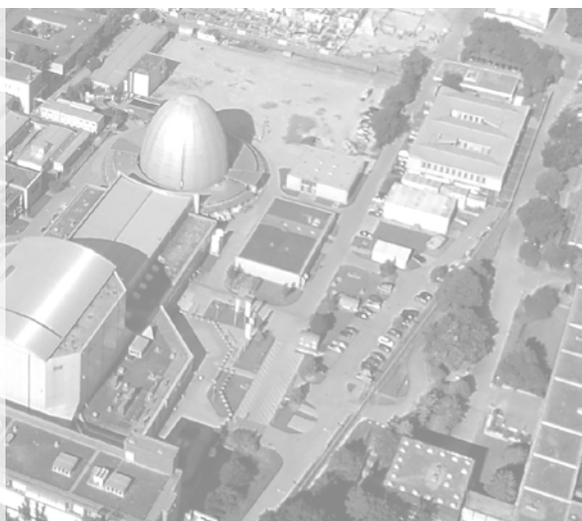
Save the Date!

SNI 2018
German Conference for Research with
Synchrotron Radiation, Neutrons and
Ion Beams
at Large Facilities 2018

will take place

at Garching

September 17th-19th, 2018!



© Ernst A. Graf

Development of a new fuel for FRM II

The need for a new fuel

Brilliant neutrons for brilliant science: Intensity per wavelength band and per angular resolution with lowest background is often decisive for the quality of an experiment at radiation sources. Users of high performance neutron sources therefore request an intense, clean neutron beam and cutting-edge instrumentation to utilise it. Such a requirement involves a continuous chain of highly specialised technologies: Culminating at the instrument, this may involve low-loss sharp energy selectors, highly reflective neutron guides and often a stable, intense cold source. The first chain-link that is common for all instruments is the reactor core, the source of the neutrons. Through this enchainment arises the need for an intense primary neutron source, i.e. a high number of fissions.

Unfortunately, such a request is contradictory to the fondness of reactor operation, the invisible but indispensable backing for excellent science at a fission-supplied neutron source. Operational and safety efforts, licensing requirements and costs grow drastically with increasing reactor power.

The elegant but powerful way out of these competing demands is the compact core concept. It combines a medium power level with a high, clean neutron flux: A single, small fuel element is placed in the centre

of a reflector with excellent moderating ratio (fig. 1). At FRM II, a large volume of D_2O provides a cloud of thermal neutrons surrounding the core. To keep the latter small, the amount of fissionable material in the pre-defined volume needs to be maximised by combining a high chemical uranium density and a high enrichment, i.e. 93% enriched U_3Si_2 dispersed in an Al-matrix with a uranium density of up to 3 g/cm^3 .

The current fuel for FRM II has proven its reliability and appropriateness for decades. Yet, changing political and societal priorities necessitate the development of an alternative fuel with significantly lower enrichment. As a part of the worldwide non-proliferation community, FRM II has committed itself to support these efforts and exchange its fuel, once a technically and economically feasible alternative is available. The development of this new fuel as well as the corresponding reactor physics calculations are the tasks of the working group "Hochdichte Kernbrennstoffe" (high density nuclear fuels).

Development requirements

A lower enrichment can be compensated by a higher chemical Uranium density. U_3Si_2 is currently limited to 4.8 g U/cm^3 , which is insufficient to get close to the ultimate goal of low enriched uranium (LEU, 20%).

Therefore, a completely new fuel based on uranium molybdenum (UMo) alloys is developed together by operators of high-performance neutron sources and fuel manufacturers from all over the world. Two options are available today, a dispersion fuel with up to 8 g U/cm^3 and a monolithic foil with up to 15 g U/cm^3 .

Developing a new nuclear fuel from scratch usually takes 20 - 25 years: The fuel needs to withstand representative irradiation tests, an industrial manufacturing process has to be developed and pre- and post-irradiation physical properties



Fig. 1: The compact core concept of FRM II: View into the D_2O moderator tank. The fuel element is located in the central channel (gold), surrounded by beam tubes (grey), secondary sources (red: converter facility for fast neutrons, blue: cold source) and safety and measurement installations (not all components are shown).

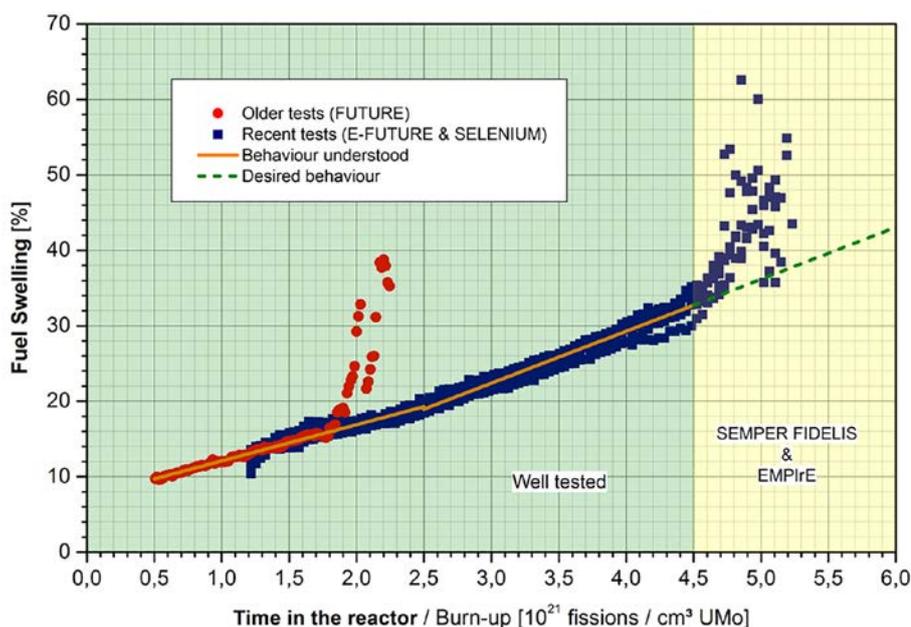


Fig. 2: Swelling of dispersion UMo fuel and progress between 2010 and 2016.

of the fuel have to be measured. Most of this R&D has to be performed with radioactive material in the strongly regulated environment of nuclear legislation. Specific for FRM II, the reactor has to be prepared for the new fuel element, where differences in geometry require reconstructions; a new safety demonstration is necessary due to altered thermal-hydraulic and neutronic properties. Care also needs to be taken about the back-end, i.e. intermediate and final storage of spent fuel as well as conditioning for final disposal. Above all of this stands the imperative to preserve the performance and safety of FRM II, for the good of science and society.

HORIZON 2020 projects

Since 2004, the R&D at FRM II is performed in a common BMBF and StMBW-sponsored project. After the foundation of the HERACLES group in 2013, the European efforts have been further generalised and merged in 2015 in the frame of the EU-financed HORIZON 2020 project HERACLES-CP. This will be further amended by the new LEU FOREvER project which has been granted by the European Commission only recently. Both projects are carried out by HERACLES, which gathers TUM, SCK•CEN, AREVA NP (CERCA), CEA and ILL.

CP means **Comprehension Phase**, and is devoted to the understanding of the unusual swelling behaviour of dispersion UMo fuels: A benign fuel swells proportional to the cumulative fission density under irradiation. Dispersion UMo, unfortunately, departs from this linear behaviour at a certain burn-up (fig. 2). The irradiation test SEMPER FIDELIS (SF) in the BR2 reactor at Belgium which starts in Sept. 2017 is designed to answer this question.

While monolithic fuel behaves well under irradiation, its fabrication is way more complex. Therefore, in SF's sister experiment in the ATR reactor, EMPIRE, monolithic UMo fuel plates that have been prepared by TUM and CERCA will be tested: Bare UMo foils that were manufactured by BWXT have been coated with Zirconium using physical vapour deposition at TUM and were then processed into plates using CERCA's new C2TWP process. The coating ensures that the fatal interaction that leads to exponential swelling (fig. 2, before 2010) is suppressed. The irradiation validation will be a milestone in the European monolithic process developments.

FOREvER will continue with the comprehension of irradiation effects, but focusses more on the further development of monolithic fuel, i.e. complex shaping to mimic FRM II's fuel density step. In addition, a back-up plan based on high density U_3Si_2 is developed in this project.

Utilising the resources from the three projects, FRM II is well prepared to take the next step from the scientific comprehension into the qualification phase once the projects have been completed. Qualification will be the final step before the actual conversion begins.

H. Breitschütz (FRM II)

More info:

www.heracles-consortium.eu

ACCELERATING Europe's leading research infrastructures

TUM-FRM II is a partner of the HORIZON 2020 project ACCELERATE. It started on Jan. 01st, 2017 and will last for 48 months. Its aim is at supporting the long-term sustainability of large scale research infrastructures (RIs) with a special focus on ERICs (European research infrastructure consortia), especially CERIC (Central European research infrastructure consortium) in Trieste, where the project is located and managed.

The project develops frameworks to improve the offer of tailored services to private and public entities, ensuring outreach to new scientific and industrial communities worldwide, and defining common protocols for monitoring and assessing RIs' socio-economic impact. A major focus on capacity building will develop current and future RIs' staff competences. The project is divided into seven work packages:

- WP1 aims at developing policies, methodologies, funding plans and human resources elements with special focus on those using the ERIC model and of CERIC specifically.
- The general objective of WP2 is the development of the RI policies, which will make CERIC more accessible to users (pilots in WP5), compliant with the Open Research Data Pilot. This includes care for harmonisation of policies in the "standard" Open Access calls being based on peer-review evaluation.

- WP3 has the goal to develop policies and procedures for commercial access, to be embodied in sets of model documents, which will be compiled in a handbook suitable for further use by other RIs. The RI partners will organise and attend a number of research-to-business events in order to build and maintain in particular with SMEs. The WP also aims at training technology transfer staff with scientific, legal, and economic backgrounds. In WP4, by using the existing contacts of its partner facilities, CERIC will identify scientific communities in European countries like Ukraine, Albania, Serbia etc., to increase its outreach.
- The WP6 (Communication and Dissemination) establishes a two-way dialogue between the project and the project's main stakeholders, as well as among the project partners themselves. The principal objective is to promote CERIC credit with stakeholders, enhance the trust of users, industrial sector, and EC as a reliable partner. In addition, these communication measures will support the exchange of best practice among RIs, both in the partnership and out.
- The WP Management (WP7) ensures the smooth execution of the project from start to the end.

TUM-FRM II will contribute to WPs 1, 2, and 6.

M. Miller (FRM II)



Participants of the Kick-off meeting visiting the ELETTRA Synchrotron facility. (© Roberto Barnabà, CERIC-ERIC)

From Serpong to Garching: exchange and education



M. Refai Muslih enjoys his stay at the MLZ.

The MLZ newsletter reports on many activities in the facility: excellent scientific results and user service, extraordinary education and training for young people, world-class instruments and their upgrades, and many others.

The MLZ also offers from time to time support for the technical programme of the International Atomic Energy Agency (IAEA), which brings together research institutions and scientists from its developing and developed member states to collaborate on research projects or training purposes. Another important support is to fund travel expenses for scientists, as many countries only have a limited budget for research activities or travels to conferences and training.

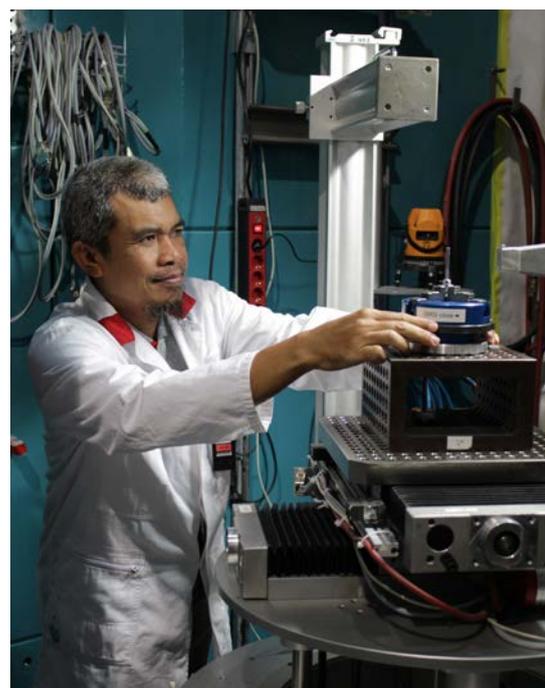
This is also the case for our guest; M. Refai Muslih from the National Nuclear Energy Agency-BATAN of Indonesia in Serpong, whose travel expenses to Garching were paid by the IAEA. Refai is instrument scientist for the DN1 (residual stress diffractometer) instrument at the GA Siwabessy Multi Purpose Reactor located in Serpong. This multi purpose reactor was designed and developed by the General Atomic company and is run with LEU at a half of full capacity of 30 MW for efficiency purposes. This capacity is e.g. adequate for research activities, isotope production for the field of industry up to health, tests as well as material testing, and science trials/experiments. "99% of the beam tubes available are for scientific purposes", Refai qualifies the official range of tasks. The 15 MW are enough for the total of seven instruments of which four instruments are connected to the reactor using two beam tubes. DN1 is quite similar to STRESS-SPEC and Refai's special interest is focussed on the NICOS software, as he wants to adapt this software to control and develop his own neutron scattering instrument in BATAN.

During his stay here in Garching he learns about set-up, measurement procedures (including data treatment) and devices used on a residual stress diffractometer as well as how to set up a personal safety system around the experimental area. He is also actively participating in the current user programme of the instrument and gains thus hands-on experience of problems encountered in performing such experiments.

In addition he will also be involved in design and development of components for the instrument control system NICOS for materials science experiments (read more about this MLZ-wide standard on page 14!). This includes training him how to protect the data taken during the experiment and operate instrument control software via a computer network. During the whole program he is being supervised by Michael Hofmann (instrument scientist at STRESS-SPEC) and Jens Krüger (head of the Instrument Control Group).

Refai Muslih stayed here for one month, but another colleague of him, Tri Hardi Priyanto, will follow him shortly afterwards. He is instrument scientist and thus responsible for DN2 (texture and single crystal diffractometer). At the BATAN facility these are two different instruments, in Garching this is the same one. His main interest will be in specialised sample environment as well as data analysis procedures and software for texture measurements.

C. Kortenbruck,
A. Voit (FRM I)



M. Refai Muslih at STRESS-SPEC.

Newly arrived

Avishek Maity



I am appointed by Georg-August-Universität Göttingen as an instrument scientist on the thermal three axes spectrometer PUMA at MLZ since April 2017.

In September 2016, I had obtained my PhD from Université de Montpellier in collaboration with ESRF, Grenoble. During this thesis work, I was mainly involved in in-situ synchrotron diffraction studies on single crystals of non-stoichiometric oxides for better understanding of low temp oxygen mobility and also the complex oxygen ordering.

I am very much interested in strongly correlated oxide materials especially to investigate versatile physical properties such as high-temperature superconductivity, charge and spin ordering / dynamics. PUMA is extremely well-suited to serve such scientific interests.

Lester Barnsley



I will be working as an instrument scientist on the small angle scattering machine KWS-1. I also plan on investigating the structure and magnetism of disordered magnetic alloys and magnetic nanoparticles.

I was previously a postdoctoral researcher at the University of Oxford, working on designs of magnetic systems for use in biomedical applications. Previous to this, I did my PhD at Griffith University in Australia, studying the magnetic properties of disordered alloys at low temperature and in high magnetic fields.

I am particularly interested in the magnetic behaviour of systems with nanoscopic features. I am also interested in understanding how magnetic structures change at extreme temperatures and magnetic fields.

Markus Kellermeier



I am the new instrument scientist at MEDAPP, the instrument for medical applications. I use the instrument for tumour therapy of patients in collaboration with the MRI of TUM. Other tasks are related to industrial use and general scientific questions.

I obtained my PhD from the FAU Erlangen, while I worked as a medical physics expert at the University Clinic. I developed a variety of clinical treatment plans and a technical-physical patient study in brachytherapy of the breast.

Neutron therapy data are a rarity and can help to understand the response of different tumours better. It is my scientific interest to track neutron interactions to gain access to their local biological effects, not just for neutron therapy alone.

Newly arrived

Monika Krug

I joined the administration-team at February 2017 and I am working together with Franziska Michel supporting Prof. Brückel, Dr. Ioffe, and the whole team of the JCNS here at Garching.

At my previous job I worked for an international company in the marketing department, especially at event management and accounting issues.



Judith Houston



In December 2016, I joined the instrument scientist team at the small-angle neutron diffractometer KWS-2.

Originally from the United Kingdom, I recently completed my PhD at Trinity College in Dublin. My research was focussed on understanding and designing systems, which self-assembled into functional materials based on conjugated polyelectrolytes and photoactive surfactants.

Going forward, I am extremely interested in building on my doctorate results to unlock novel, smart materials for future energy generation and storage devices.

Dmitry Gorkov



I am the new instrument scientist working on the construction of KOMPASS, the upcoming three axes spectrometer at MLZ.

I did my PhD at Ruhr University Bochum, where I worked on development of time-resolved polarized neutron reflectometry technique (TRAC-PNR) for study of magnetisation dynamics in thin films and nanopatterns.

My research interest besides the TRAC-PNR is the investigation of behaviour of magnetic NPs in AC-magnetic field and their interaction with biological lipid membranes in view of hyperthermia applications.

Kerstin Koch



I am responsible for the Bio- and Chemistry Lab and for sending dangerous goods - that means, I support users in these labs. Thus, I take care for the lab safety as well as for the crystallisation of proteins.

Before, I had worked at the Helmholtz Centre in Neuherberg at the research unit environmental simulation (Institute of Biochemical Plant Pathology). I measured VOC with GC-MS and PTRMS. I was also responsible for the evaluation of the data. I also did the technical support for the LC-MS.

I am looking forward to learn more about crystallisation and about the measuring of those crystals!

The UCN group



Fig. 1: The members of the UCN group.
Front (f. l. t. r.): T. Deuschle, C. Bocquet, S. Wenisch, W. Adler.
Back: J. Schilcher, A. Frei, S. Wlokka.

Neutrons are an excellent tool to probe matter and investigate its properties. Mainly thermal or cold neutrons are used as such probes. If neutrons have energies below approx. 300 neV, they are termed **ultra-cold neutrons (UCN)**. Such neutrons can be stored in special material or magnetic bottles, and can therefore be observed for long time periods (several tens of minutes). In such experiments with UCN, the neutrons itself are the particles which are investigated with respect to their structure and their behavior in neutron decay.

Precision experiments with UCN, such as the search for a possible **electric dipole moment (EDM)** of the neutron or the measurement of the lifetime of the free neutron, require high UCN densities. Stronger UCN sources are presently developed worldwide, based on the principle of superthermal UCN production, using cryo-converters made of solid deuterium (sD_2) or superfluid helium. At the FRM II, a UCN source with a sD_2 converter and sH_2 pre-moderator, placed in a distance of ~ 60 cm from the central fuel element inside the horizontal, through going beam tube SR6, is currently under construction. It can generate UCN densities of $\sim 10^4$ cm $^{-3}$ in up to four connected experiments. These densities are more than two orders of magnitude higher compared to the currently strongest UCN source at the ILL.

The central part of the UCN source is the converter vessel, a double walled toroidal shaped aluminium cap piece, which is cooled by a continuous flux of a closed supercritical helium cooling loop. The necessary cooling power of 1.0 kW at 5 K is supplied by two cold boxes (AirLiquide Helial 2000) to the closed supercritical He-loop. The converter contains 12.5 mol of solid hydrogen (sH_2) as pre-moderator (volume ~ 250 cm 3) to pre-cool the incoming thermal neutron flux ($\sim 10^{14}$ cm $^{-2}$ s $^{-1}$) to an effective neutron temperature of ~ 40 K. The sD_2 UCN converter (maximum amount 12.5 mol) is frozen to the outer surface of the converter vessel by re-sublimation of D_2 gas to the solid phase. The pre-moderated incoming neutrons can enter the sD_2 converter, where they excite solid state excitations (mainly phonons) of the crystal lattice. Solid ortho-deuterium has excited states in the energy range of 2 - 20 meV, so that by populating one single excited state by neutron scattering at the crystal lattice, the incoming neutron loses practically its total initial energy, and is converted into the energy regime of ultra-cold neutrons. The UCN generated by this process can leave the sD_2 converter, and are guided to the SR6 beam port exit in the Experiment Hall, and fed into connected experiments.

The task of the UCN group (see fig. 1) is to construct and implement all parts of the source together with all needed auxiliary systems in the existing reactor facility. Besides the central parts of the source mainly different cooling systems, media supply systems, media release systems and control and data acquisition systems are needed to operate the UCN source.



Fig. 2: Newly built housing to the south of the MLL for the He-compressors of the UCN-source, with two helium gas tanks (on the left) and a liquid nitrogen tank (on the right).



Fig. 3: Left: A 1:1 rebuild of the SR6 beam tube of the FRM II. Right: The control station of the test set-up. Back: The cold boxes of the cooling system.

Hereby all parts, that are constructed and built up at the FRM II, have to fulfil conventional and nuclear regulations. Additionally, the operation of the UCN source with the media hydrogen and deuterium is considered as a major change to the licensed state of the reactor, and therefore requires a complete licensing according to nuclear law.

The process of nuclear licensing includes a non-nuclear test phase with prototypes of all parts of the UCN source. During the last year such a test setup of all important components of the UCN source has been installed at the Maier-Leibnitz-Laboratory (MLL). Three vessels, one filled with liquid nitrogen and two filled with gaseous helium, have been set up outside south of the MLL building. A 70 m² wide and 3.70 m high hall made out of wood houses the two compressors (electrical power 250 kW each) of each cold box accompanied by two oil separators and water filled circuits for the cooling of the compressors (see fig. 2). A small cooling tower next to the compressor hall removes the produced heat from the water cooling circuits. The helium cooling machines themselves are located inside the Maier-Leibnitz-Laboratory. Two conventional cooling machines with a power of 500 W at 5 K each remove the heat from a closed cooling cycle of supercritical helium. Each machine expands the previously compressed helium using seven heat exchanger stages (the first stage precooled with liquid

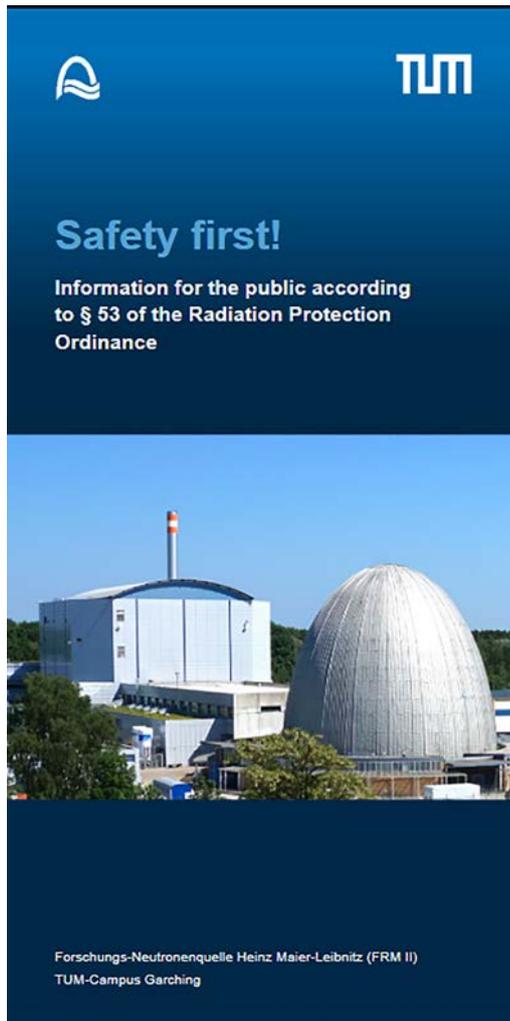
nitrogen) and two expansion turbines to produce liquid helium in two vessels in the third cold box. The liquid helium is then used to cool a closed loop of supercritical helium via two heat exchangers. This closed loop, which is driven by a special pump, is connected with cryogenic transfer lines to a small vessel inside of the SR6 beam tube, housing the solid deuterium and the solid hydrogen.

A 1:1 rebuild of the beam tube SR6, where all the converter parts of the UCN source stay, has been set up (see fig. 3). The helium cooled converter vessel is placed in the middle inside the beam tube SR6. For non-nuclear tests the heat input of the FRM II to the converter is simulated by several heating devices.

With all these systems the UCN source has now started its non-nuclear test phase. In these tests all parameters how to operate the cooling machines and all necessary auxiliary systems will be varied and optimised in order to freeze out deuterium and hydrogen in a dedicated way, with the simulated nuclear heat load of the FRM II. After the tests, which will take approximately one year, the whole cooling machine, together with the helium and liquid nitrogen vessels, will be transferred to the FRM II, and all the other parts of the source and auxiliary systems will be built and installed.

A. Frei (TUM)

New brochure “Safety first”



According to §53 of the German Radiation Protection Ordination the FRM II is obliged to produce and distribute every five years a new information brochure for the immediate neighbours of the Garching campus. This brochure was completed in time in 2013, but retrieved because the authorities had to revise the civil protection. This took about two years because the district administrator had a lot of work to organise everything for the refugees in 2015. At the end of 2016 the brochure was finalised, the signature of the (in the meantime) new district administrator was on hand and we could print several thousand issues of the new brochure “Safety first” in March 2017.

It contains useful information for the population in the surrounding of the FRM II. The research neutron source was already constructed with strict security requirements, e.g. the walls are built with 1.80 m thickness of heavy concrete and the reactor pool is

completely separated from the surrounding building. Even for the purely hypothetical case of a partial or complete nuclear melt the reactor building itself would be an effective radiological protection. Taken into consideration were, among other things, the effects of floods, a complete power failure, earthquakes, plane crashes – even of large commercial airliners – and assumed malfunctions such as the hypothetical case of a partial or complete meltdown.

Readers learn a lot about the physical details of how the reactor works and the whole safety concept of the FRM II, which is constantly controlled. A further information block presents the details of the civil protection of the Munich district. In case of a disaster the population would be warned via loudspeaker, radio, television, videotext, and internet or via the smartphone app “Katwarn”.

For the first time an English version is now available as a printed issue which therefore considers the grown international population in the surrounding of the FRM II. The MLZ itself has more than 1000 users a year, many of them coming from abroad and also do the other TUM facilities and Max-Planck-institutes on the campus Garching. Several thousand international students also stay permanently on the campus and live in the surrounding.

The new brochure is effective until March 2022 and can also be downloaded on the FRM II webpage. It will then be fundamentally revised, maybe in even more languages?

C. Kortenbruck, A. Voit (TUM)



Do you like to have a look? Just download the English version by using the qr-code!

Next Proposal Deadline: September 08th, 2017

Find all information at

- mlz-garching.de/englisch/user-office/getting-beam-time.html



Submit your proposal at

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

Next Rapid Access Deadline: July 28th, 2017



Tobias Unruh

Chairman of the 10th
Komitee Forschung mit Neutronen
(KFN)

Tobias.Unruh@fau.de

Dear friends,

the term of the 10th KFN will expire soon and responsibility will be taken over by the elected members of the 11th KFN in autumn 2017. So, it is time to take a short moment for reflection and look back on the work of the KFN in the last two election periods.

It was in October 2011 when I took over the chair of the 9th KFN. It was the time when an intense discussion about the strategy for setting up the European Spallation Source in Lund, Sweden was taking place. The KFN strengthened the participation of the German user community in the selection process of the first ESS instruments, tried to integrate German universities and research facilities in the development of instrument proposals, and contributed strategy papers for the science case of the ESS and the necessity of a strong German contribution.

Finally, the German government agreed to contribute 10% of the total building and operation costs of the ESS. This is less than claimed by the KFN but it paved the way for the begin of the ESS construction phase.

The happiness about the building of the ESS had been overshadowed by the unexpected decision of the HZB to fully stop its engagement in operation of neutron instruments with the shut down of the BER II reactor at the end of 2019. It was and is a continuous task of the KFN to support the operation of neutron instruments at and by the HZB and I do hope that the new scientific management of the HZB will reconsider the HZB strategy for neutron instrumentation.

The KFN attended the signing of the 5th protocol of the ILL, the 10 years anniversary of FRM II, the founding of MLZ, several HZB and FRM II user meetings and is engaged in ENSA, KEKM, IRI, and RACIRI. We co-organised three SNI/DN meetings and could decorate three Wolfram-Prandl-Prize winners. Another major effort of the KFN was to provide to the BMBF recommendations for the calls for proposals of the collaborative research. It also supported the idea of the evaluation of the collaborative research initiative. In the final evaluation report the great effectiveness and success of this unique funding scheme became obvious which is a great success of this BMBF funding initiative.

It would certainly go beyond the scope of this short address to count up all the many activities of the KFN in the last years, so many of them have not been mentioned. However, I will not end without having expressed my deepest gratitude to the members and the co-opted members of the 9th and 10th KFN and the representatives of the neutron research centres for their support and the tremendous efforts they invested for the benefit of the German neutron community. I also have to thank the BMBF, the project management organization at DESY, and the neutron research centers for the efficient and trustworthy cooperation. Many thanks also to the excellent support of Karin Griewatsch in 20 KFN meetings and for her activity in all organisational things, web design, and public relations for the KFN.

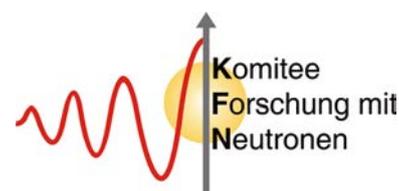
Although significant goals have been reached, a lot of challenges need to be addressed by the 11th KFN. A coordinated initiative of the different user committees with the large scale facilities for the digitalisation offensive of the national government (big data, scientific data management) needs to be worked out. It is of outstanding importance for the German user community that an initiative for a new national neutron source (replacing the capacity of the BER II source) has to be set on track. Furthermore, the elongation of ILL operation needs to be accomplished in order to achieve several years of overlap with a fully operational ESS. Finally, a roadmap for the implementation of a European network of national neutron research facilities and the ILL/ ESS as flagship neutron sources has to be established. This includes a European programme for transnational access to national neutron sources.

Although these challenges are very demanding, I am convinced that they will be perfectly met by the 11th KFN for which a list of candidates with highest reputation could be assembled. I have to thank all the candidates for their willingness to continue the work of the KFN which is essential for the future of German research with neutrons.

Finally, I would like to thank the whole German user community for your confidence and support over the last six years. With the best wishes for a bright future of the research with neutrons in Germany, Europe, and the world -

yours sincerely

Tobias Unruh



Use of MLZ beam time 2016

In the year 2016 the reactor operated two cycles (N. 39 and N. 40 of 60 days each) for a total of about 3.108 instrument days delivered.

The largest fraction was used for research, both for external and internal users, which used about 80% of the total instrument days. The MLZ instruments are operated mainly for the benefit of external users, who can perform an experiment only if their submitted proposals are positively assessed by the international MLZ Review Panel. For each internal experiment performed at the MLZ instruments, about two experiments of external users are carried out.

The remaining instrument days were used for many different and very important tasks:

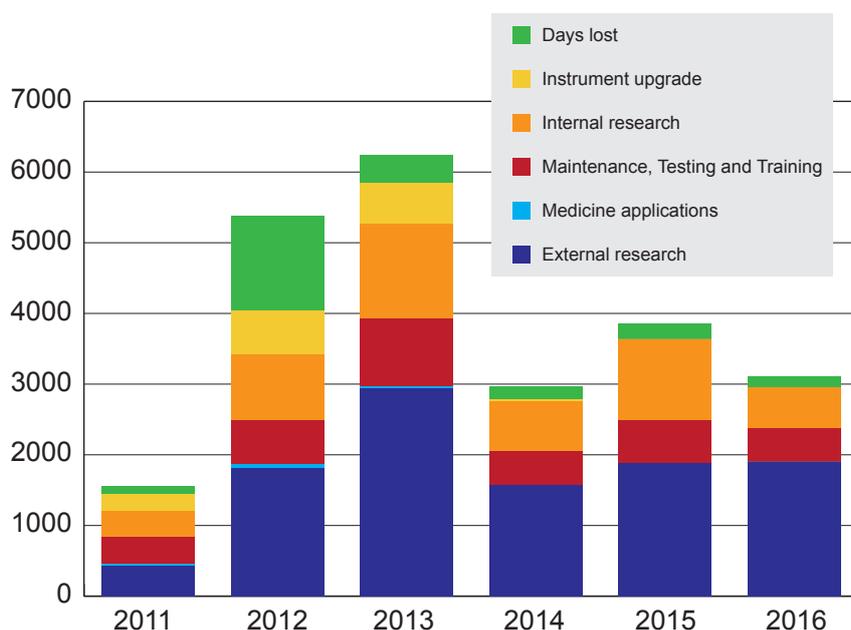
- industrial and medicine applications, where the use of the MLZ instruments is of the interest of industries and of patients for medical treatments (0.4% of the total instrument days)
- training of young scientists, with the organization of several labcourses where the students can work hands on the MLZ instruments and acquire a valuable expertise for their future career (2.5% of the total instrument days)
- the MLZ instruments have to be always kept up-to-date for the benefit of the research users, for their research usage as well as for their development with new technical possibilities (12.6% of the total instrument days)

The MLZ is a sophisticated technical facility and it is unavoidable to have needs and technical problems that reduce the use of the instruments. In the year 2016, the beamtime losses due to different failures and instrument unavailability were very low (about 5%); they were very well managed by the MLZ instrument scientists and staff members, on duty round the clock to react promptly at the smallest problems affecting the completion of an experiment. Due to the construction of the new neutron guide hall east, a very valuable investment for the future with six additional instruments available for the user operation, one instrument was out of operation because it had to be dismantled, moved and rebuilt with a new neutron guide. This very delicate task was accomplished in one reactor cycle only, i.e. about 60 instrument days.

In the figure the evolution of the use of the MLZ beam time is shown for the last six years.

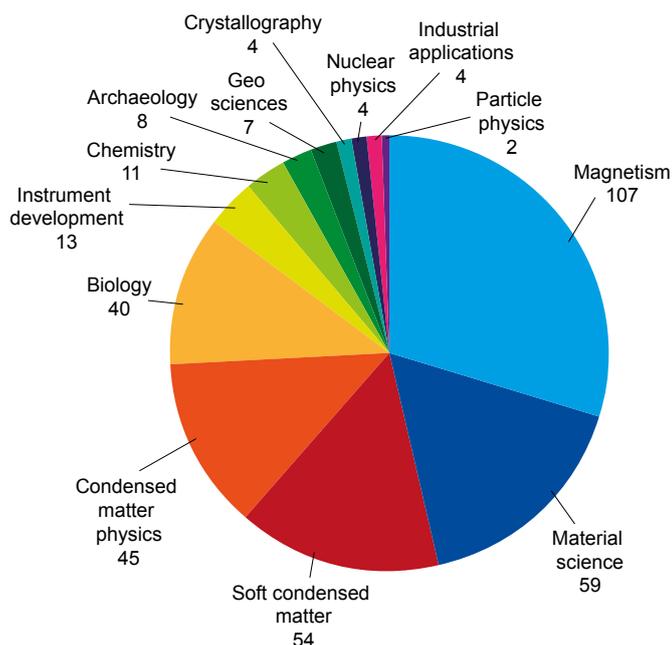
The number of beam days delivered to external research is the second highest absolute value since 2011. However, due to the lower total number of instrument days delivered in 2016 compared to 2013, its fraction is by far the highest in the last six years. Moreover, the beam time losses in 2016 are the second lowest absolute value, however its fraction is the lowest in the same period.

F. Carsughi (JCNS)



Use of the MLZ beam time in the years 2011-2016.

MLZ proposal round 2017-I



Scientific fields of the submitted proposals

The submission deadline for the first proposal round in 2017 was on January 27, when 358 proposals were submitted to the 27 available MLZ instruments, for a total of 2.341 beam days requested, with an increase of about 16% compared to the last proposal round.

The largest fraction of the proposals (about a half) have been submitted by scientists of German institutions, with an increase of about 6% compared to the last proposal round, about one third by the European colleagues, with an increase of about 19%, and, surprisingly, about 15% by the Asiatic ones, with an increase of more than 76%.

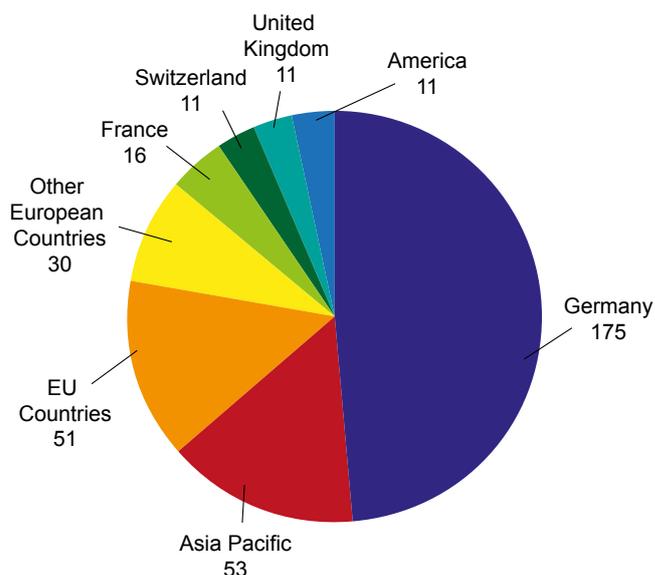
The MLZ instruments are mostly demanded for investigations in magnetism, material science, soft condensed matter, condensed matter physics and biology, leaving about 15% to the other scientific topics.

The review panel meeting took place on March 8th and 9th, where the members meet to discuss on the submitted proposals and rank them according to their recommendations to the MLZ Directors. Missing experimental reports were also considered for the final ranking approved by the MLZ Directors.

A total of 1.554 beam days were allocated and 261 proposals were accepted. The small angle scattering

diffractometer KWS-2 and the positron spectrometer NEPOMUC are the most requested instruments in terms of proposals, 34 and 31, respectively, while in terms of beam days the neutron reflectometer N-REX and the positron spectrometer NEPOMUC were the most demanded ones with 145 and 142 requested days, respectively. The neutron reflectometer N-REX and the diffractometer for large unit cell BIODIFF have the largest overbooking factor 2.6 and 2.3, respectively, being the overall MLZ overbooking factor 1.6.

At the MLZ a waiting list for the best rejected proposal has been established, and it includes 30 proposals on 13 different instruments. These waiting list proposals can be accepted once all the other accepted proposals have been measured and additional beam time will become available in the proper time frame at an instrument. The MLZ User Office informed the waiting list applicants and will turn them to the accepted status whenever the conditions mentioned above will be fulfilled.



Country of origin of the submitted proposals

We welcome four new members in four different MLZ Review Panels and are very grateful to those who terminated their membership. The whole MLZ Review Panel provides an extremely important work for the scientific community.

F. Carsughi (JCNS)

Upcoming

International Conference on Neutron Scattering 2017

July 09 - 13, Daejeon (Korea)

www.icns2017.org/

Visit our booth there!

Hydrogen School 2017

Aug. 07 - 17, Berlin (Germany)

www.helmholtz-berlin.de/events/hydrogenschool/index_en.html

IAEA Training Workshop: Advanced Use of Neutron Imaging for Research and Applications: AUNIRA

Aug. 28 - Sept. 01, Garching (Germany)

webapps.frm2.tum.de/indico/event/51/

21st JCNS Laboratory Course - Neutron Scattering 2017

Sept. 04 - 15, Jülich + Garching (Germany)

www.neutronlab.de

MATRAC 1 Autumn School

Sept. 25 - 29, Ammersbek + Hamburg (Germany)

www.hzg.de/ms/summerschool/058651/index.php.en

JCNS Workshop 2017

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

Oct. 10 - 13, Tutzing (Germany)

fz-juelich.de/jcns/JCNS-Workshop2017

NINMACH 2017 - 2nd International Conference on Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage Research

Oct. 11 - 13, Budapest (Hungary)

indico.kfki.hu/event/518/overview

Save the Date of the SNI 2018!

Sept. 17-19, 2018, Garching (Germany)

Reactor Cycles 2017

No.	Start	Stop
41	24.01.2017	24.03.2017
42	03.05.2017	01.07.2017
43	08.08.2017	06.10.2017

Imprint

Editors

Rainer Bruchhaus

Flavio Carsughi

Christine Kortenbruck

Ina Lommatzsch

Jürgen Neuhaus

Andrea Voit

Layout and typesetting

Ramona Bucher

Ina Lommatzsch

June 2017

Picture credits

Cover

W. Schuermann, TUM

Back cover

Henn GmbH

Contact

Forschungs-Neutronenquelle

Heinz Maier-Leibnitz (FRM II)

User Office

Lichtenbergstraße 1

85747 Garching, Germany

Phone: +49.(0)89.289.10794

10703

11751

Fax: +49.(0)89.289.10799

e-mail: useroffice@mlz-garching.de

www.mlz-garching.de



© R. Demmel (TUM)

The Remains of the Day...

