

Newsletter

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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 Science and the Arts and the partners of the cooperation.

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Looking back: looking ahead

Outstanding performance, excellent ideas for future developments, and a very strong potential for expanding into new application areas were some of the key words we identified during the review of the MLZ in November last year. Chairing this review has been a pleasure and a duty for me. The detailed results of the review were presented to the steering committee of the MLZ in May 2019.

The evaluation covered not only the past four years of operation, having a look at the performance of the instruments and organisational and management issues, but as well on the future plans of the MLZ for the next ten years. All of this was presented in detail in a printed book and discussed during our interesting stay on-site in Garching in November 2018. On behalf of the review panel, I would like to thank all the staff and students at MLZ for having prepared their presentations and posters so well. This clearly demonstrate your strong engagement. In the review panel we were only sorry that we did not have more time to discuss all the interesting science you presented.

It is clear that the MLZ with its long-term perspective will certainly continue to play an important role in the European and international landscape of neutron providers, especially in the actual changing situation in Europe. Based on the excellent properties of the neutron source FRM II, with dedicated moderators for cold, thermal, hot, and fast neutrons and an intense source of positrons, several instruments are unique and the best, or among the very best, in their class on an international level. This potential could even be better exploited in a broader range of applications if appropriate resources were available, especially for the staffing level. This holds true even more for the ambitious plans to increase the number of user instruments and upgrade initiatives to address the changing requirements of the scientific community.

Strategically and in practice, MLZ plays a very central role as one of the leading European neutron sources and one of the top-5 international sources. Indeed, it is hard to imagine the international neutron landscape without the MLZ.

*An editorial
by*



*Lise Arleth
(University of Copenhagen)
Chair of the MLZ Review Committee*

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USER OFFICE

Physics with positrons@MLZ

High-intensity positron beams, i.e. with at least 10^7 monoenergetic positrons per second, are generated via pair production using high-energy gamma radiation [1]. In the late 1980s, Klaus Schreckenbach came up with the idea to use neutron capture gamma-rays for electron-positron pair production at a reactor. In 1998, we started to design the NEutron-induced POsitrone source MUniCh (NEPOMUC) based on the nuclear reaction $^{113}\text{Cd}(n,\gamma)^{114}\text{Cd}$ as an in-pile component inside the moderator tank of FRM II. As shown in fig. 1, the positron beam is magnetically guided to five different instruments, where the kinetic energy is usually varied between 20 eV and 30 keV.

Revealing point defects with unprecedented sensitivity

The workhorses for depth dependent defect spectroscopy are the instruments PLEPS and CDBS. PLEPS (developed at the Bundeswehr University Munich) allows the measurement of the positron lifetime as function of implantation energy. This in turn enables the analysis of various defect types and their concentration. Examples are the identification of Sr and Ti vacancies in thin film SrTiO_3 or vacancies in thin solar cells of compound semiconductors. Furthermore, PLEPS allows the characterisation of the free volume in amorphous materials such as thin film polymers.

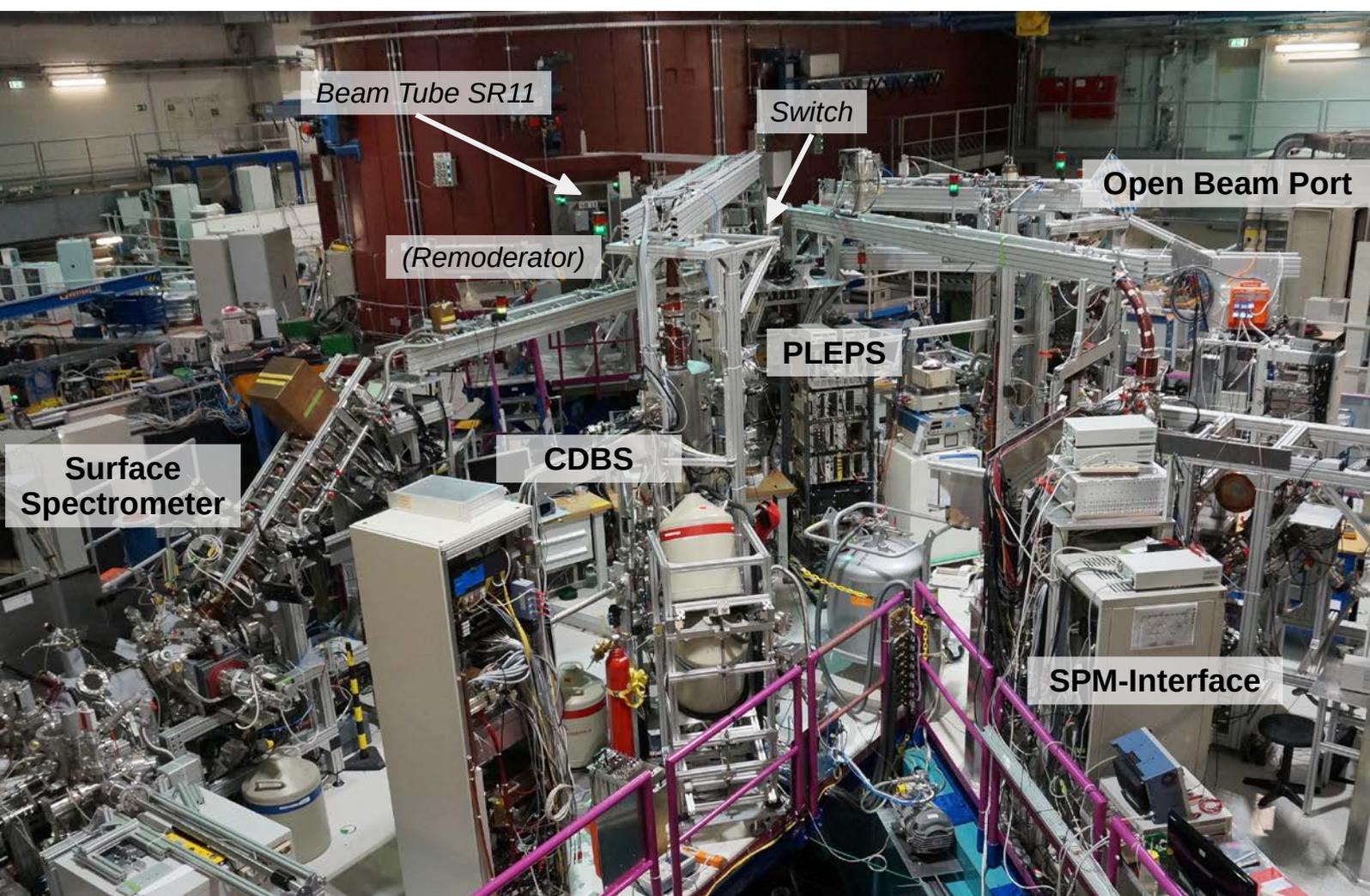


Fig. 1: Positron beam facility at NEPOMUC in the Experimental Hall: The positron beam generated inside beam tube SR11 is magnetically guided via a remoderator for brightness enhancement and a beam switch to various instruments: (i) surface spectrometer for positron annihilation induced Auger electron spectroscopy (PAES), (ii) coincident Doppler broadening spectrometer (CDBS), (iii) the pulsed low-energy positron system (PLEPS), (iv) an interface for a scanning positron microscope (SPM), and (v) an open beam port for additional experimental set-ups.

At the CDBS, the Doppler-shift of the annihilation photons is detected providing insight in the electron momentum distribution of the sample. Moreover, the scanning positron microbeam at the CDBS enables laterally resolved measurements in two dimensions with a resolution below 50 μm ; the third dimension is accessible by variation of the positron implantation energy. This feature is particularly interesting for verifying the structural homogeneity of samples. The main application is hence imaging of defect distributions and the analysis of the chemical surrounding of open volume defects, e.g. impurities forming foreign atom-vacancy complexes. Examples are the investigation of lattice defects in electrode materials for Li-ion batteries, irradiation induced damage of technical alloys or the influence of vacancies and antisite disorder to the magnetic phase transitions e.g. in MnSi. Recently, we studied the defect distribution around a laser beam weld of the high-strength age-hardenable Al alloy AlCu6Mn by laterally resolved DBS. Additional CDBS was applied with unprecedented spatial resolution to reveal the dissolution of Cu rich precipitates and the formation of Al-vacancy-Cu-complexes in the weld nugget [2].

High temperature superconductivity with a maximum transition temperature (T_c) of 92 K in $\text{YBa}_2\text{Cu}_3\text{O}_{(7-\delta)}$ (YBCO) is strongly influenced by the oxygen deficiency δ . The local T_c in YBCO thin films (200 nm grown by pulsed laser deposition on STO substrates) has been analysed with spatially resolved DBS. It was shown that DBS is particularly suited to investigate oxygen vacancies in YBCO since the positron probes the plane with the relevant Cu-O chains [3]. The S-parameter (see fig. 2) as a measure of the Doppler-broadened annihilation line is correlated to the oxygen vacancy concentration of the sample. The YBCO thin film samples showed a large variation of T_c between 20 and 90 K. Note that the variation of T_c can be revealed within the individual samples.

Topmost layer surface analysis

The specific interaction of positrons with surfaces enables experiments with topmost layer sensitivity for the investigation of both, the element distribution at the surface and the surface structure. Positron annihilation induced Auger electron spectroscopy (PAES) is particularly suited for non-destructive element selective surface experiments. In contrast to conventional Auger-electron spectroscopy (AES) using X-rays or keV-electrons (EAES), at PAES the core shell ionisation is induced by the annihilation of positrons with core electrons. Therefore, the energy of the primary positron beam can be chosen considerably lower (~ 10 eV) than the typical electron energy (\sim keV) in EAES. As a consequence, PAES exhibits exceptional surface sensitivity and besides, the secondary electron background in the range of Auger-transition energies is suppressed.

In Cu-Pd alloys, the amount of Cu atoms and their spatial distribution can significantly affect the mechanical stability and the catalytic properties of thin Pd membranes. Density functional theory calculations predicted the migration of Cu in the second atomic layer of Pd. The high beam intensity at NEPOMUC allowed us to apply time-dependent PAES for the investigation of the stability and dynamics of thin layers comprising a few mono-layers of Cu on the Pd surface. For the first time, the migration of Cu atoms in the second atom-

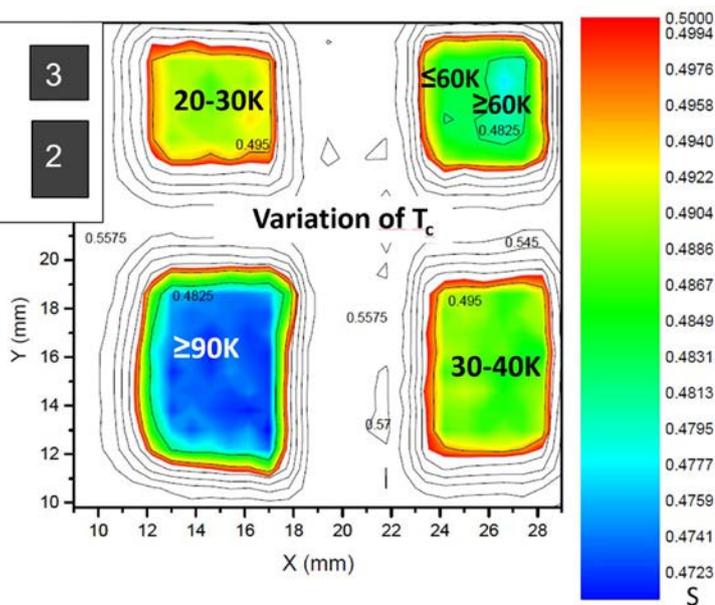


Fig. 2: 2D-S-parameter map of four 200 nm thin YBCO samples obtained by spatially resolved DBS (positron energy: 4 keV). The variation of the S-parameter (colour code, right) allows the determination of the local T_c inside the individual samples.

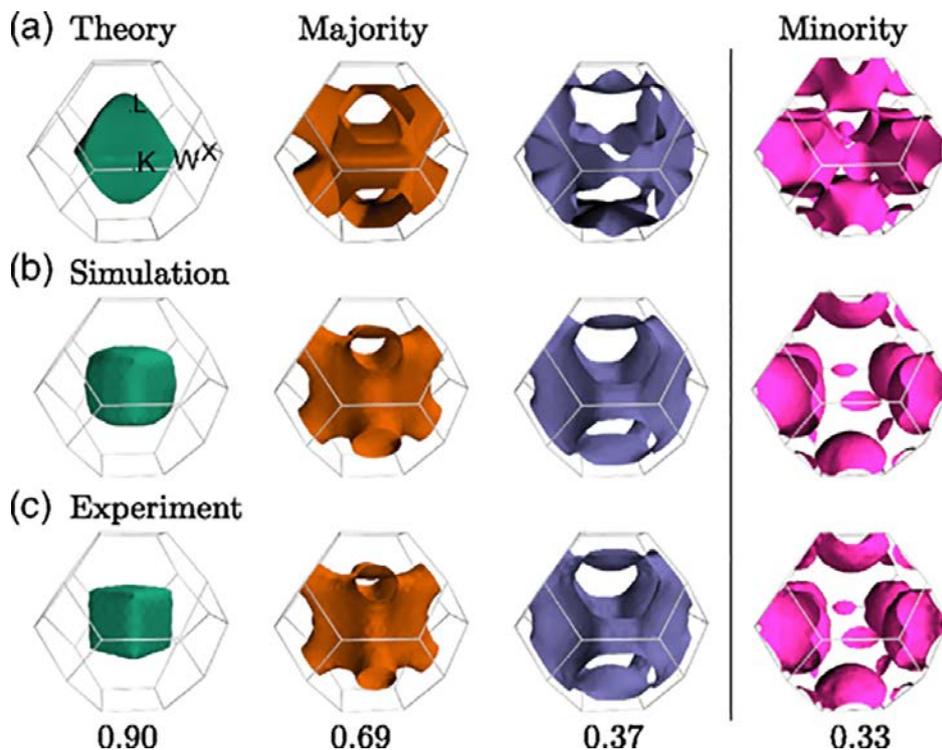
Fig. 3: Majority (left) and minority sheets (right) of the Fermi surface of Cu_2MnAl : (a) fixed spin moment ($3.2 \mu \text{B/f.u.}$) calculations, (b) reconstructed simulated data convolved with the experimental resolution function including statistical noise, and (c) isosurfaces of experimental data. The occupied fraction of the Brillouin zone volume of the experimentally determined Fermi surface is given below each sheet [4].

ic layer of Pd was observed in situ. For the segregation process, a characteristic time of 83 min was found by analysing the temporal change of the Cu and Pd Auger intensities.

Diffraction experiments for surface structure analysis showed that for positrons total reflection occurs for small incident angles due to the different crystal potential whereas for electrons it is not observed. Using total-reflection high-energy positron diffraction (TRHEPD) the structure of reconstructed surfaces, e.g. of TiO_2 [1], could be determined with highest precision. In order to benefit from the high positron intensity a positron diffractometer is currently being set up for first TRHEPD measurements at NEPOMUC.

Gaining insights in correlated systems using spin-polarised positrons

A powerful experimental technique providing unique information about the bulk electronic structure is the measurement of the two-dimensional angular correlation of electron-positron annihilation radiation (2D-ACAR). At the Maier-Leibnitz-Laboratorium (MLL), we perform 2D-ACAR measurements using a ^{22}Na source which emits longitudinally spin-polarised positrons owing to parity violation in the weak interaction. Since in metals the electron-positron pair annihilates overwhelmingly in the spin singlet configuration, the different spin channels of a ferromagnet can be examined by applying magnetic fields. A prominent example is the determination of the spin-resolved Fermi surface of the prototypical Heusler compound Cu_2MnAl (see fig. 3).



The three-body problem and the pair plasma – Fundamental research with leptons

The positronium negative ion Ps^- is a bound system consisting of two electrons and a positron. About 50 years ago, Wheeler discussed the stability and bound states of “polyelectrons” such as Ps^- . The ground state of Ps^- is stable against dissociation but, naturally, unstable against annihilation into photons. Since the constituents are point-like leptonic particles of equal mass Ps^- is a three-body system par excellence and hence an ideal object to study the quantum mechanics. Furthermore, the production, acceleration of Ps^- and subsequent photo-detachment would pave the way for the creation of an energy-variable (neutral) Ps beam.

Within a collaboration of TUM, LMU, and MPI for Nuclear Physics, a tabletop tandem accelerator was set up at NEPOMUC using two 5 nm thin diamond-like carbon foils for production and acceleration of Ps^- . The ground-state decay rate of Ps^- could be determined with unprecedented accuracy to $2.0875(50) \text{ ns}^{-1}$ in

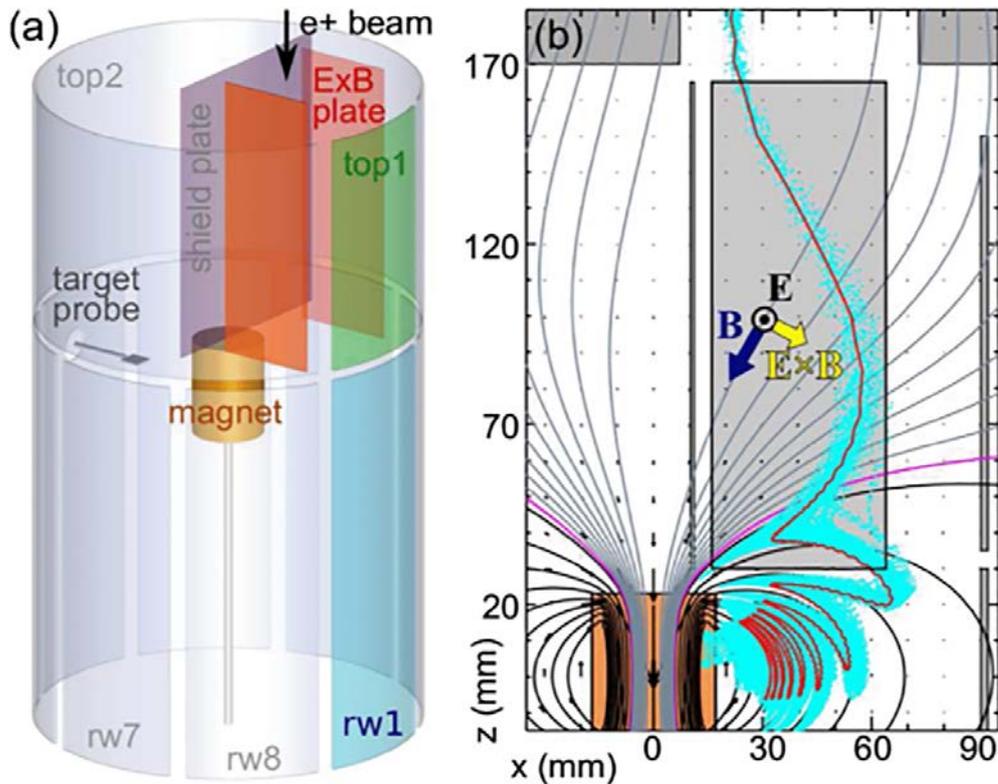


Fig. 4: (a) The experiment set-up for confining a pair plasma. (b) A typical simulation of lossless $E \times B$ transport from field lines connecting to the beam line (top) and into the confinement region. Points along the trajectories of 100 particles are projected onto the xz plane (cyan dots), as is a single trajectory (red line) [6].

agreement with recent theoretical predictions from quantum electrodynamics calculations [5].

Trapping of an electron-positron plasma in a laboratory set-up would enable novel studies of pair plasmas. Such plasmas are assumed to occur in the vicinity of neutron stars and black holes and are predicted to have properties significantly different from those of standard electron-ion plasmas. A fundamental challenge, however, is the development of a facility that allows efficient injection and confinement of both electrons and positrons. In the current experiments at NEPOMUC a dipole field of a simple permanent magnet is used to trap positrons (see fig. 4). The APEX collaboration aims to create a pair plasma on earth for the first time. Within this collaboration, an injection efficiency of 100 % was achieved. In addition, positron confinement times in the magnetic dipole trap of more than one second have been observed for the first time [6]. In order to considerably increase the trapping time further the current setup will be replaced by a new chamber housing a levitated superconducting coil for positron and electron confinement.

Financial support from the Deutsche Forschungsgemeinschaft (DFG projects HU 978/15-1, HU 978/16-1, SFB-TRR 80) and from the Bundesministerium für Bildung und Forschung (BMBF projects 05K13WO1 and 05K16WO7) is gratefully acknowledged.

Summary

The unprecedented intensity of low energy positrons provided by NEPOMUC lead to a tremendous improvement of the signal-to-noise and a considerable reduction of measurement times for a wide range of applications. Moreover, for fundamental research completely new positron experiments have been implemented for the first time. In the near future we aim to produce ultra high dense positron pulses paving the way for first experiments on positron-positron interaction.

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Read more

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- [2] T. Gigl et al., New J. Phys. 19 (2017) 123007.
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KWS-2: Control of the incoherent background via TOF-SANS

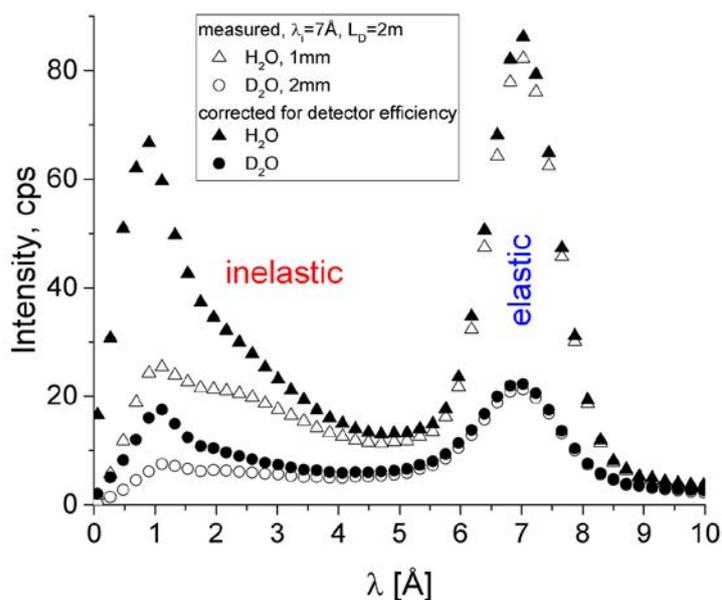


Fig. 1: The TOF spectra from H₂O and D₂O recorded at KWS-2.

In a small angle neutron scattering (SANS) experiment one measures the coherent scattering which bears the structural information about the sample and is predominantly elastic, and the Q-independent incoherent scattering. The incoherent “background” from hydrogenated systems contains a significant amount of inelastic scattering that is not negligible, as usually considered in SANS [1]. Inelastic scattering occurs at high Q and adds to the scattering signal at small angles as a result of multiple scattering. In this case the incoming monochromatic neutrons are thermalised in the sample and scattered with higher energies than the incoming (monochromatic) ones, hence with shorter wavelengths.

The amount of this inelastic scattering that is detected in a SANS experiment depends on the detector efficiency at short wavelengths. One should take proper care of this incoherent inelastic scattering when subtracting the “incoherent background”, especially in the case of weakly and coherently scattering systems in dilute solutions. The incoherent component from the solvent sample that is used for background subtraction differs from that of the sample of interest, due to the solute. Moreover, the measured incoherent scattering is considerably larger than the calculated one based on the known sample composition [2]. Therefore, in order to control the incoherent background due to inelastic multiple scattering, it is useful to equip

the SANS instruments with an option that operates with a pulsed monochromatic incident beam and time-of-flight (TOF) data acquisition.

Recently at the high intensity SANS diffractometer KWS-2, we had commissioned a compact chopper that can be installed in front of the sample on demand. This single-disc chopper that is pulsing the incoming beam and triggers the TOF data acquisition has four windows with fixed opening of 1 cm and can operate at selected frequencies within the range 15 to 50 Hz in order to match the TOF conditions for a given incoming neutron wavelength λ_i and detection distance L_D .

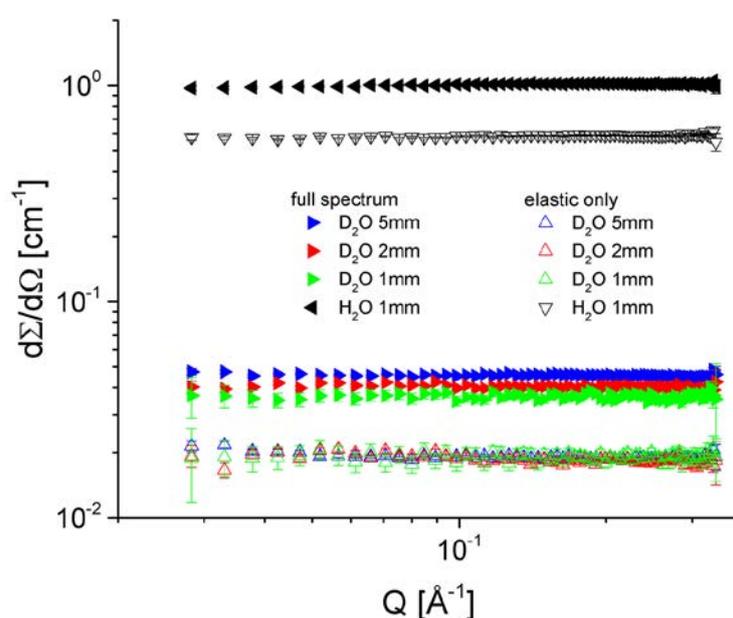


Fig. 2: The measured scattering cross section of H₂O and D₂O when full scattering spectrum or only the elastic scattering are considered.

Our tests showed that a good separation of the inelastic from the elastic scattering can be obtained in case of hydrogenated or deuterated samples (fig. 1). Considering only the elastic component for the data analysis, we can reduce the incoherent background from diluted systems (fig. 2) and detect more accurately weak coherent signals from proteins or polymer chains in solutions.

A. Radulescu, L. Balacescu,
G. Brandl (JCNS)

Read more

[1] A.R. Rennie & R.K. Heenan, proceedings of ISSI Meeting, Dubna 1992

[2] A. Brulet et al, J. Appl. Cryst. 40, 165, 2007.

Taming neutrons at SPHERES

The SPectrometer for High Energy RESolution (SPHERES) at MLZ is a third generation backscattering spectrometer with focussing optics and phase-space transform (PST) chopper. It provides high energy resolution with a good signal-to-noise ratio. Over the years several components of the instrument had been upgraded to further improve the instrument's performance.

Some recent years ago, the PST chopper had been renewed.

The new more compact one-wing chopper can be operated with the desired speed close to the optimum velocity for the phase space transformation and has new graphite deflector crystals on its circumference with higher reflectivity and mosaicity. Thanks to the increased velocity and the better deflector crystals, the intensity in most detectors had been doubled.

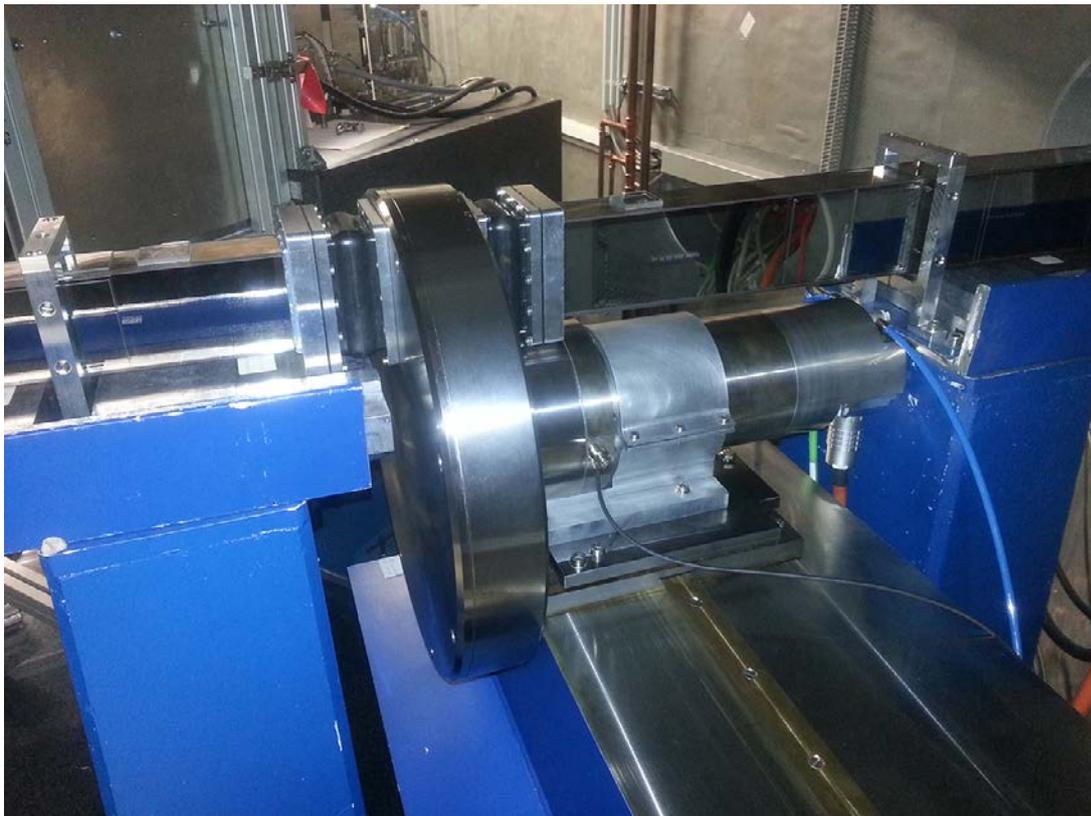


Fig. 1: The new focussing neutron guide with the background chopper.

Last year the linear convergent “anti-trumpet” neutron guide had been replaced with a focussing guide with double elliptical shape (vertical and horizontal). It had been optimised based on McStas simulations which also considered the new PST chopper. With the new elliptic guide another intensity gain at the sample position of about 30 % was obtained.

Together with the exchange of the focussing guide also a new background chopper had been installed (see fig. 1). It is situated about 2 m upstream of the PST chopper to further reduce background. In regular operation, the signal-to-noise ratio for typical samples is about 2000:1. Spinning the background chopper at half the speed of the PST chopper it also allows for a high signal-to-noise set-up by eliminating every second pulse, albeit at the cost of intensity. In a first test experiment a signal-to-noise ratio of about 12000:1 was obtained (see fig. 2). In particular absorbing samples with low signal could profit from this low background mode.

M. Zamponi, M. Appel, D. Noferini (JCNS)

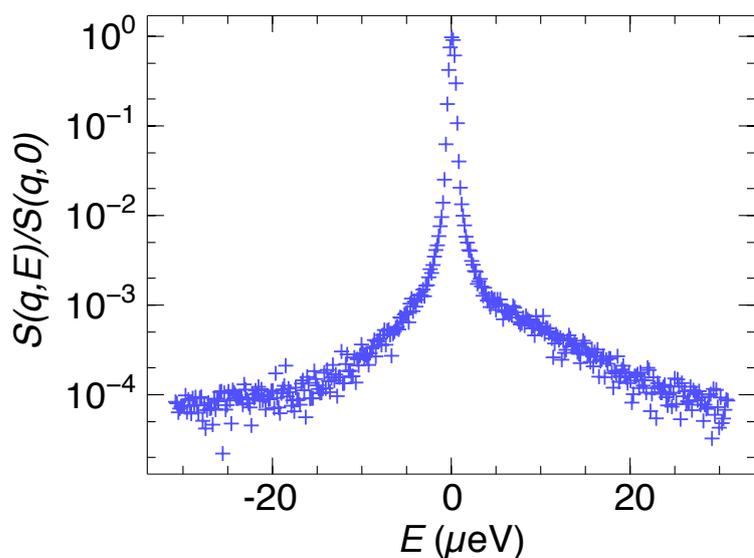


Fig. 2: Resolution function for a polymer sample for the high signal-to-noise set-up.

In situ light scattering and absorption: Complementary techniques to SANS at KWS-2

Understanding of soft and biological materials requires the global knowledge of their microstructural features from elementary units at the nm scale up to larger complex aggregates in the micrometer range. Such a wide length scale can be explored at the KWS-2 small angle neutron (SANS) diffractometer of JCN5. Additional information obtained by in situ complementary techniques plays sometimes a very important role for an increased reliability in the SANS analysis of systems undergoing structural modifications under external stimuli (temperature, solvent pH, humidity, illumination, etc.) or which are stable only for short times. Observations at the local molecular level structure and conformation help for an unambiguous interpretation of the SANS data using appropriate structural models, while monitoring of the sample condition during the SANS investigation ensures the sample stability and desired composition/chemical conditions. Thus, we equipped KWS-2 with complementary light absorption and scattering capabilities.

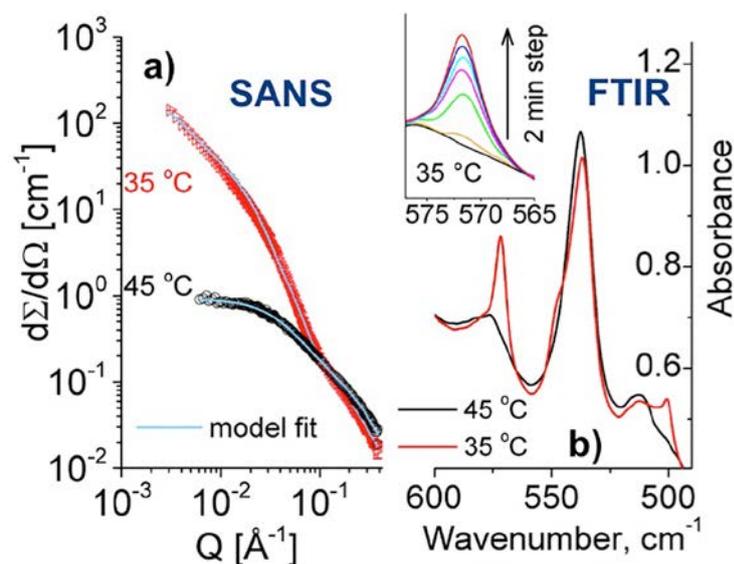


Fig. 1: Example of simultaneous SANS and FTIR analysis.

UV/Vis and Fourier transform IR (FTIR) spectroscopy can now be performed simultaneously with standard and time-resolved SANS. The gelation of syndiotactic polystyrene (sPS) from solution in decreasing temperature could be understood in detail (fig. 1a,b) following this approach: the sPS shows an amorphous chain conformation at 45 °C, while at 35 °C it is in a helical conformation, as revealed by the evolution of the characteristic IR band at 572 cm^{-1} . Accordingly, the

SANS data could be described by using the semi-flexible single chain and the interconnected platelets form factors. Special optics allow for the sample to be hit simultaneously by light and neutron beams, either co-axially (the in situ FTIR set-up) or perpendicularly (the in situ UV-Vis approach).

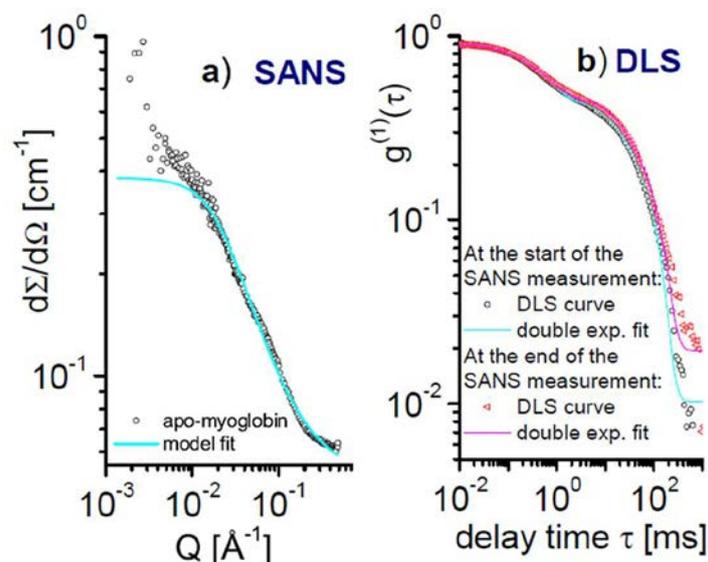
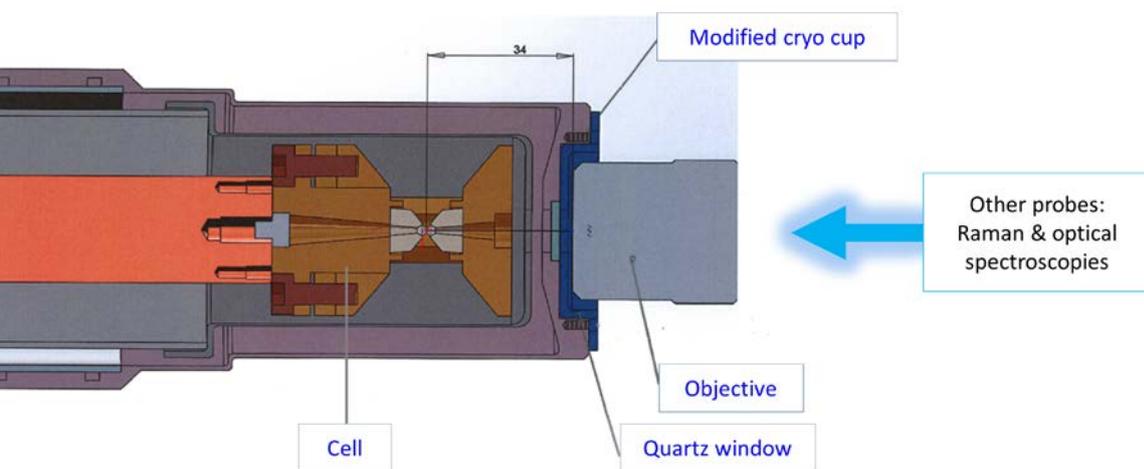
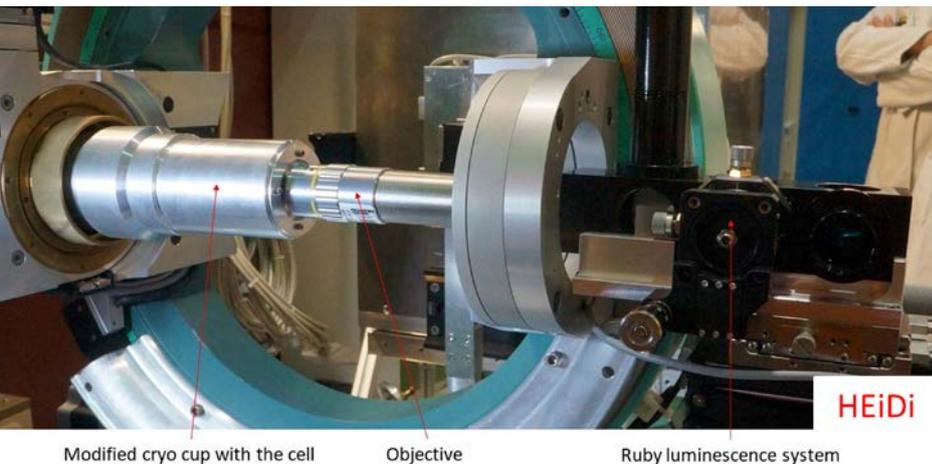


Fig. 2: The SANS curve of the molten globule state of apo-myoglobin (a) with in-situ DLS data (b).

Moreover, in situ dynamic light scattering (DLS) became available for routine experiments, which enables to observe either changes in the sample composition, due to sedimentation effects, or in size of morphologies, due to aggregation processes. This has consequences in beam time organisation (abandon the current measurement on the unstable sample and start it over again with a fresh sample) and data reduction optimisation (disregard the SANS data at some point or consider the large scale aggregates of a size revealed by DLS in the SANS modeling procedure). In fig. 2, the DLS curve at the beginning of the SANS experiment matches the one at the end. Aggregates are present in both curves. Their size can be inferred from a double exponential fit of the DLS curve giving a hydrodynamic radius of 1370 nm. In the SANS data only at very low Q some data points point to aggregates being present in the sample. Those data points can therefore be ignored in the model fit of the protein scattering data.

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High pressures and small samples on HEiDi



Low-temperature set-up at HEiDi.

Within the current BMBF project “Extension of the Hot Single Crystal Diffractometers HEiDi for Experiments on Small Samples $< 1 \text{ mm}^3$ and with High Pressure Cells” (05K16PA3), the instrument HEiDi at the hot source of FRM II undergoes a major hardware upgrade. The optimised neutron optics includes a new Cu220 monochromator to increase the neutron flux (gain factor > 2) and solid-state collimators that, together with a parabolic neutron guide will result in a small beam size at the sample position with a high signal-to-noise ratio.

These improvements will allow studies on crystals with sizes comparable to those used for standard X-ray diffraction (crystal volumes well below 0.1 mm^3). This achievement offers the benefit

of combined neutron and X-ray diffraction studies on exactly the same samples and the extraction of neutron specific information not achievable with X-rays, for instance, magnetic structures and hydrogen bonding.

In-situ high-pressure single-crystal diffraction has been introduced at HEiDi recently. Various high-pressure diamond anvil cells (DAC) have been developed (panoramic and transmission cells) and first data collections using them are performed [1]. All cells are made of non-magnetic materials, including the Ni-Cr-Al alloy with very high strength, no neutron activation and very weak neutron attenuation [2].

The panoramic DAC offer a large opening angle and can be placed in the modified cryostat with an optical window. Pressure changes with temperature are followed with ruby luminescence. The new low-temperature set up allows temperatures down to 3 K and can be useful also for combining neutron diffraction with spectroscopic experiments (e.g., Raman and optical spectroscopies). Transmission DAC are suitable for both neutron and X-ray diffraction. The membrane cell type can be operated remotely changing its pressure via a He gas filled membrane. The same crystals in the same cells were studied on HEiDi as well as on the laboratory X-ray diffractometer IPDS-II in Aachen and on the synchrotron beamline P24 (Chemical Crystallography) at Petra-III in Hamburg. We are now working on the proper procedure to combine the neutron and X-ray data sets for joint refinements of the crystal structure.

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Read more

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March 31st- April 05th: DPG Spring Meeting



Once again the DPG Spring Meeting of the Condensed Matter Section was held at Regensburg! The

weather was not that bad for the beginning of April, but it was no reason for the nearly 5000 participants mostly from Germany not to flock to one of the 3127 talks and have a closer look at a total of 1399 posters. Last but not least, a lot of them also visited the MLZ booth for a quick chat and liked our ballpoints that much that they created a work of art using them (see fig.)...

At the booth, we could announce the next proposal deadline on September 13th as well as the upcoming annual MLZ Conference – this year, it deals with neutrons for information and quantum technology. Furthermore we were also happy to distribute the freshly printed advertising cards for the next MLZ User Meeting here at Garching on December 10th-11th. See you there!

I.Lommatzsch (FRM II)



March 28th: A future day for girls – become a scientist!

30 girls show up for the Nationwide Girls' Day at the MLZ to find out how to become a "scientist". They have an infinite number of questions.

First, TUM-scientist Johanna Jochum talks about a typical working day at the neutron source. Before we search for the scientists, there is a short excursus on radioactivity.

Can one see radiation and is it dangerous? We have brought an experimental case, with which the girls can examine e.g. uranium-containing tiles, watches with ¹⁴⁷Pm luminous dials as well as garden fertilizer - radiation from natural sources.

And what does radiation actually look like? We stop at the cloud chamber. The girls can actually see thick short alpha particles and even long thin beta-particles.

What do the scientists actually investigate with neutrons? The eyes of the girls sparkle as we explain the experiment with the 70 million year old Dino eggs.



© W. Schürmann (TUM)

So many instruments, but where are the scientists? We meet them in the corridors, offices and finally also in the laboratories. Chemical-technical assistant Tabea Bartelt and PhD student Livia Balacescu (both Forschungszentrum Jülich) let the 13 and 15 year olds measure the pH value in liquids, observe crystal growth under the microscope, weigh substances with a scale. In the end, the girls leave with a bag full of give-aways and the wish to become a scientist themselves.

A. Görg (FRM II)



April 08th- 10th: PARI 2019 – Workshop on communicating science

It's not every day that science communicators from across the globe can be in the same place for stimulating discussions and exchanging best practices.

The Public Awareness of Research Infrastructure (PARI) conference was hosted by the Rutherford Appleton Laboratory. For over 100 delegates, the three-day programme hoped to inspire individuals to make complex information well understood to the public and distribute it as broadly as possible.

Tori Blakeman, STFC's Impact and Engagement Officer said: "The three days I spent at PARI 2019 were stimulating, inspiring and hugely enjoyable. I loved taking part in lively debates with science communicators from all over the world and gaining insights into communications tactics from many world-leading organisations." MLZ press officers Anke Görg and Andrea Voit were sharing their knowledge in a workshop on "Video training: How do I successfully communicate my key message in a crisis". Some of the hot top-



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The workshop dinner took place at the Formula 1 Williams car exhibition.

ics during the conference were discussing fake news, LGBTQ+ representation in STEM and the importance of unconventional outreach.

PARI 2019 was supported by EIROforum and ERF-AISBL Association of European-level Research Infrastructure Facilities.

ISIS/ STFC



Feb. 24th- 27th: SAAGAS

The conference series "Seminar on Activation Analysis and Gamma Spectrometry" (SAAGAS) was originally introduced by Franz Lux at TUM in 1970. This year in February, the 27th SAAGAS returned to its place of origin.



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After the conferences in Aachen (2015) and Vienna (2017), C. Stieghorst of the MLZ PGAA group organised the conference in co-operation with the German Chemical Society (GDCh). Around 70 scientists from more than ten countries met in Garching and discussed the recent developments and applications in the field of neutron activation analysis, gamma spectrometry and related methods.

The presentations of the participants covered a wide range of applications - hot topics were e.g. archaeometry, battery research, analysis of food and environmental samples, nuclear waste or astrophysics. New methodological developments were also presented. Highlights were the invited talks of R. Henkelmann (itg), G. Korschinek (TUM) and H. v. Philipsborn (Universität Regensburg). M. Trunk and L. Werner (both TUM) received the GDCh young speaker's award for their talks about Neutron Depth Profiling (NDP).

C. Stieghorst (FRM II)



Nov. 23rd, 2018: Women in Nuclear

In the end of 2018, the general meeting of WiN Germany was held at MLZ Garching. Women in Nuclear is an organisation of women (and in some countries men) working professionally in nuclear energy, technology and radiation applications, worldwide organised in WiN Global. The day before, the participants visited the facility (guided by W. Lohstroh and A. Schneidewind), impressed about the technical performance of the facility and its instruments, and surprised about the huge variety of scientific use and its impact to society. In the evening, discussions continued, but also moved to the topics of gender equality and female career. The talk by R. Güldner focussed on the ten years anniversary of WiN and highlighted the role of successful women in this field.

In the general meeting itself A. Schneidewind, B. Pollum, E. Krapf, and T. Huber presented their development which finally lead to a work at MLZ, followed by the presentation of the winner of the 2018 WiN Ger-



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many Award, B. Schacherl (KIT) about “Structural investigation of Np interacted with illite by HR-XANES and EXAFS”. Finally, in an internal session, the formal association’s work was done: reports, elections and further plans. WiN Germany is a lively network with access to a broad part of technological, political and scientific aspects of nuclear technique and application. The members use the meetings to visit different places related to their working fields, and moreover – we thank them for their interest and the intense, fruitful discussions.

A. Schneidewind (JCNS)



March 31st- April 05th: MATRAC-2 School



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The MATRAC 2 School 2019 – Application of Neutrons and Synchrotron Radiation in Materials Science with Special Focus on Fundamental Aspects of Materials (www.hzg.de/summerschool) took place in Hirsching and Garching with 40 students from eight different countries. A systematic overview of the application of neutrons and synchrotron radiation in the structural analysis of materials including all relevant scattering

and imaging methods was given in a three-day theoretical course. The presentations by fifteen experts ranged from the basics of elastic and inelastic scattering of neutrons and X-rays to details of experimental techniques to modern functional materials. During two poster sessions, the participants presented their work and there were lively scientific discussions between the participants and the lecturers of the school.

During the two-day course with “hands-on” experiments at the MLZ instruments, each participant had the possibility to work at two different neutron instruments in a short and a long experiment (with a following detailed analysis). The students demonstrated the results of their long experiments and evaluations in short presentations on the school’s last day.

The students’ feedback on the school was very positive. In particular, the practical experiments were highly appreciated and the commitment of the scientists of the MLZ instruments was highlighted.

N. Kampner; K. Pranzas, S. Busch, M. Müller (HZG)



March 26th: Launching LENS

On March 26th, 2019 members of a strategic consortium of neutron research facilities in Europe, the League of advanced European Neutron Sources (LENS), officially launched activities to promote collaboration on common issues like neutron usage, technology development, and data.

By aligning policies among its partners, LENS will advocate for the user community and strengthen European neutron science. The members of LENS held their first General Assembly and the first Executive Board meeting in Liblice, the Czech Republic. The consortium adopted and signed statutes detailing the purpose of LENS and laying the framework for working groups responsible for the execution of foreseen activities. The signing ceremony was followed by a public event that celebrated the launch of LENS in the presence of around 80 government representatives, national delegates to the European Strategy Forum on Research Infrastructures (ESFRI), the European Commission, and the wider scientific community.



The event also featured panel discussions about the long-term sustainability of neutron sources, and the various ways in which neutrons contribute to excellent science and advance innovation. As a collaborative effort that aims to benefit researchers and address their needs, LENS established good working relations with the European Neutron Scattering Association (ENSA).

J. Neuhaus (FRM II)



Jan. 14th- 15th: BrightnESS² Kick-off Meeting 2019



The three-year programme BrightnESS² is a European Union-funded project within the European Commission's Horizon 2020 Research and Innovation programme and had its kick-off meeting in January.

The kick-off took place prior to both the annual meeting of European Neutron Scattering Association (ENSA) delegates, and discussions hosted by the League of Advanced European Neutron Sources (LENS), an in-

itiative launched last year to strengthen collaboration among neutron facilities.

BrightnESS² is in alignment with the activities of both ENSA and LENS, thus enforcing the bridge between users and research facilities that generate neutrons. Over the course of 36 months and with a budget of nearly 5 Mio€, BrightnESS² aims to support a long-term sustainability of the European Spallation Source (ESS), its user community, and the network of neutron sources in Europe.

Alongside 14 international research organisations, the Heinz Maier-Leibnitz Zentrum (MLZ) participated in a European neutron science project to build a neutron ecosystem for sustainable science with the ESS. BrightnESS² is composed of a total of six work packages, and the MLZ will contribute to three of them, specifically supporting the development of a European neutron strategy in a global context.

A. Fröhner (FRM II)

Dear colleagues,

Even while waiting for fuel elements, spring 2019 is not boring. We work on our publications, instrument scientists maintain and upgrade their instruments. MLZ scientists have a chance to think strategically – about new instruments, about better support, about use of all the new technologies which are already available or will come up in the nearest future. One of these upcoming topics will be the digital transformation. The user representations of ErUM communities KAT, KET, KfB, KFN, KFS, KFSI, KHuK, and RDS were asked by BMBF to develop a strategy for it. The results are condensed in the document “Challenges and Opportunities of Digital Transformation in Fundamental Research on Universe and Matter. Recommendations of the ErUM Committees” which was delivered to BMBF on May 2nd, 2019. The strategy document reflects all the needs and requirements that the different communities are facing – and the work on it could be the initiation of a long-term cooperation to accomplish these challenges across the different disciplines.

A second road of support is the DFG initiative “NFDI – National Research Data Infrastructure” which will be established as a cooperative network of consortia to ensure systematic management of scientific and research data. KFN and MLZ are working towards active participation in one of these consortia, to ensure the realisation of digital infrastructure at MLZ, ILL, and ESS in the users’ interest. In all these processes, the collaboration of KFN and KFS is further developed and intensified in order to exploit the synergies of comparable methods.

Making use of synergies, cooperate where things are better done together than separately is also the aim of the LENS initiative. In March 2019, the activities were launched officially. Working groups were installed to allow the specialists to organise their collaboration in the best way and we are looking forward to lively discussions to define best practices. In some fields, SINE2020 work packages, ISSE etc. may give an excellent starting option.

Cordially,
Astrid Schneidewind

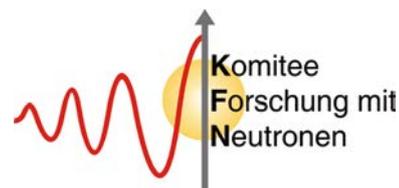


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Astrid Schneidewind

Chair of the 11th KFN
(Komitee Forschung mit Neutronen)

a.schneidewind@fz-juelich.de



Investigation of binary Zr-Ti melts processed by electromagnetic levitation (EML)

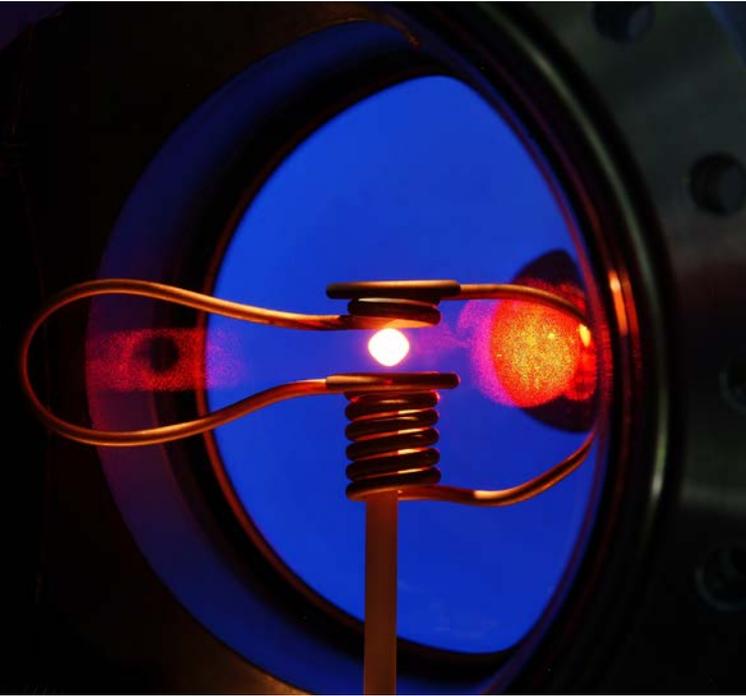


Fig. 1: Levitating metallic droplet, processed by electromagnetic levitation (EML).

Knowledge on the properties of metallic melts is essential to understand the solidification of metals. During the transition from the liquid state to a crystalline state, atoms form a long-range ordered system, emerging from a disordered system. Here, the atomic transport mechanisms in the liquid phases play an essential role. However, processing of some metallic melts is rather challenging, due to the respective temperatures and the chemically highly reactive nature of metallic melts, e.g. sample-container reactions and oxidation. Containerless-processing of melting metallic samples by an inductive coil (see fig. 1), so called electromagnetic levitation (EML), became a utile technique to investigate such melts.

In electromagnetic levitation, contamination and nucleation from the container are suppressed and in-situ investigations of different kinds of metallic samples are possible. In stationary EML the density, the undercoolability, the nucleation, the surface tension, and the solidification behaviour of metallic melts are investigated.

To obtain high quality viscosity data, measurements under well-defined experimental conditions in micro-gravity using the TEMPUS facility aboard parabolic

flights and the MSL-EML on the Columbus Module of the International Space Station (ISS) are possible. In addition, the electrical resistivity can also be determined.

Furthermore, a mobile EML had been designed by the Institute of Materials Physics in Space of the German Aerospace Center (DLR), which serves as a sample environment for large scale facilities to carry out scattering experiments, e.g. at MLZ.

One example is at the multi disc-chopper time-of-flight spectrometer TOFTOF (see fig. 2), where quasielastic

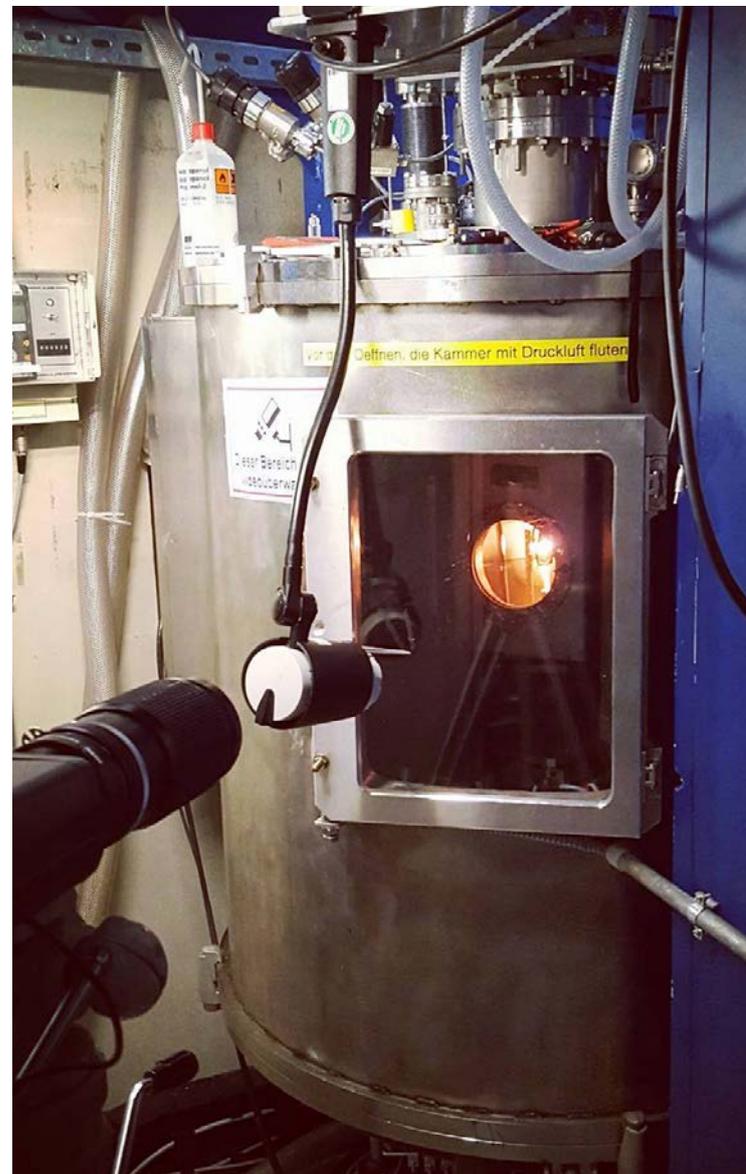


Fig. 2: Electromagnetic levitator (EML) of DLR installed at TOFTOF.

neutron scattering (QENS) experiments can be performed in order to study atomic transport processes, e.g. self-diffusion. Samples with sizes of 6-8 mm in diameter can be processed in a broad temperature range from 1000 K to 2500 K. Thus it allows detailed investigations of the liquid state down to the deeply undercooled state for metallic elements and alloys.

Neutrons enable a detailed microscopic probing of structure and dynamics in liquid-state due to their wavelength, which is comparable to typical interatomic spacing of 1-2 Å, and with energies similar to excitation energies in condensed matter. Quasielastic neutron scattering provides simultaneously information on the structure (from the momentum transfer) and dynamics (from the energies gain/ loss of the scattered neutrons) of the melt.

As an example, binary Zr-Ti melts were investigated. Zr and Ti are of the same early-transition metal group in the periodic table. Alloyed they compose a completely miscible system, which is the binary boundary system for many bulk metallic glasses (BMGs), e.g. Zr-Cu-Ti, and stable quasi-crystals, e.g. Zr-Ti-Ni. For these systems a relevant impact of chemical short-range order (CSRO) on the liquid dynamics is reported. Fig. 3 shows a dynamical structure factor $S(Q, \omega)$ of liquid $Zr_{50}Ti_{50}$ at a temperature of 1930 K measured at the TOFTOF instrument. The broadening of the elastic line (FWHM) gives direct access to the self-motion of atoms. Since QENS probes atomic motion directly on a pico-second time scale, which is not affected by any convective flow, this allows a determination of the diffusion coefficient on an absolute scale with errors typically smaller than 5%. Its high neutron flux and very low instrumental background make TOFTOF ideal for carrying out such experiments with small samples.

In fig. 4 self-diffusion coefficients of Zr-Ti melts measured utilising EML at TOFTOF are depicted. The experimental error bars are on the order of the symbol size. Due to the element specific incoherent scattering cross-sections ($\sigma_{Ti} = 2.87$ barn, $\sigma_{Zr} = 0.02$ barn) only the motion of Ti-atoms in the melt is measured. The self-diffusivity of Ti follows an Arrhenius behaviour over the entire investigated temperature range. At a given temperature the liquid self-diffusion coefficient

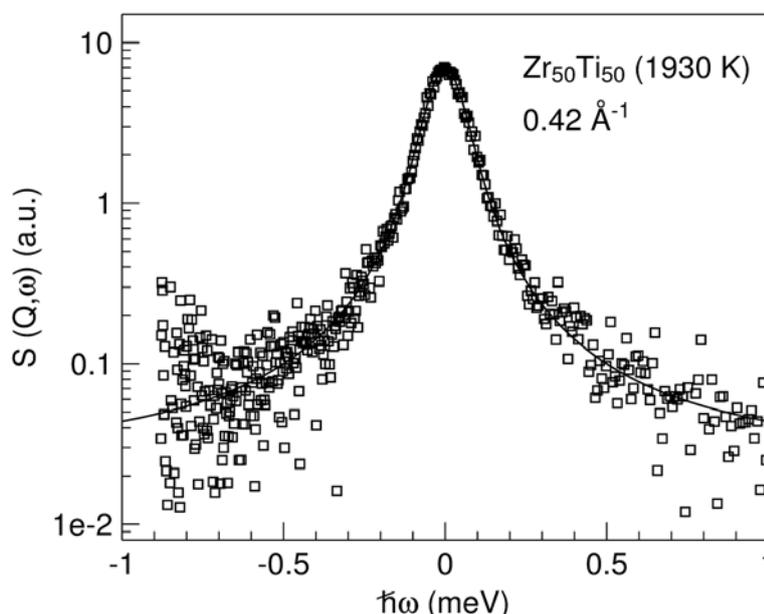


Fig. 3: Dynamical structure factor $S(Q, \omega)$ of liquid $Zr_{50}Ti_{50}$ at 1930 K at a momentum transfer of $q = 0.42 \text{ \AA}^{-1}$.

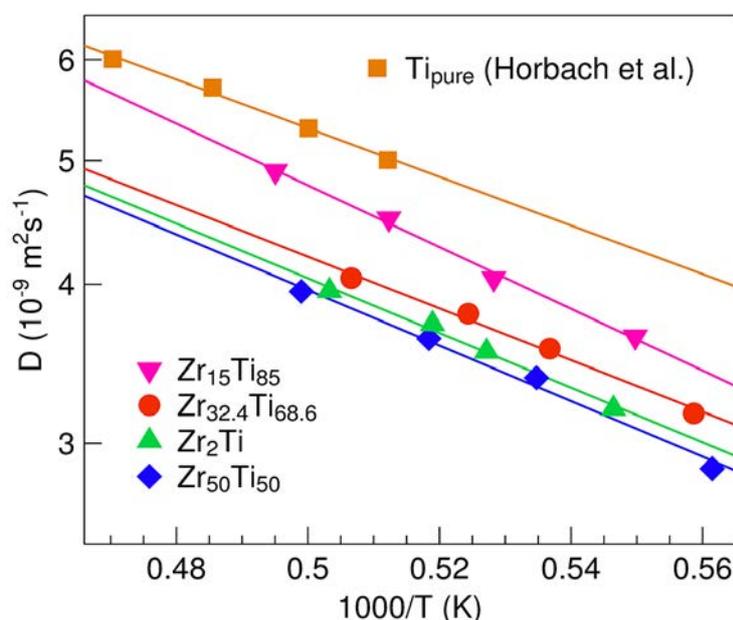


Fig. 4: Self-diffusion coefficients of Ti in Zr-Ti melts, measured using electromagnetic levitation at TOFTOF.

of the investigated alloys decreases with increasing Ti content. Similar characteristics can be described considering a simple hard-sphere model, where only the topology of atoms is reflected. In-situ neutron diffraction shows that barely any chemical short-range order (CSRO) is present in Zr-Ti melts and the structure is indeed dominated by topological packing. This is in line with our results of the concentration dependent change in diffusivity.

S. Szabo (FRM II)

Delivering neutrons for research, industry and medicine: Life cycle of a fuel element



The fuel element of the FRM II is a hollow cylinder of some 1.3 m in length, 24 cm diameter and with a total weight of 53 kg. It contains approximately 8.1 kg of uranium enriched to 93 % of the fissile uranium ^{235}U . The fuel in use is U_3Si_2 dispersed in Al.

Looking closer at it, the fuel element contains 113 separate fuel plates which are

Fig. 1: Fuel element for FRM II.

mounted between an inner and an outer tube with diameters of 118 mm and 237 mm respectively. Because of the fuel element's compactness, the moderation of the neutrons takes place in the surrounding heavy water tank. An effect that made it necessary to decrease the fuel density in the outer part of the plates from 3 g/cm^3 to 1.5 g/cm^3 in order to avoid an unacceptable power peak at the outer surface of the fuel element. The fuel plates are bent to an involute shape in order to guarantee cooling slits of constant width namely 2.3 mm. The cooling is established by light water being pumped through the cooling slits at a rate of 300 kg/s (11 bar) and leading to a temperature increase of the cooling water of only about 15 K, i.e. from $\sim 35 \text{ }^\circ\text{C}$ to $\sim 50 \text{ }^\circ\text{C}$.

Fabrication of FRM II fuel elements

The uranium comes from Russia and the fresh fuel elements are manufactured in a production plant in France (Framatome/CERCA). The common picture frame technology is used for the plate fabrication:

1. Fusion/Grinding: Uranium metal is melted with silicon to obtain a uranium alloy. The alloy is then milled into an extremely fine powder over several steps.
2. Pressing/Framing: Next, the powder is compressed into a core, which is then inserted between an aluminium frame and cover plates to form a pre-plate or "sandwich."

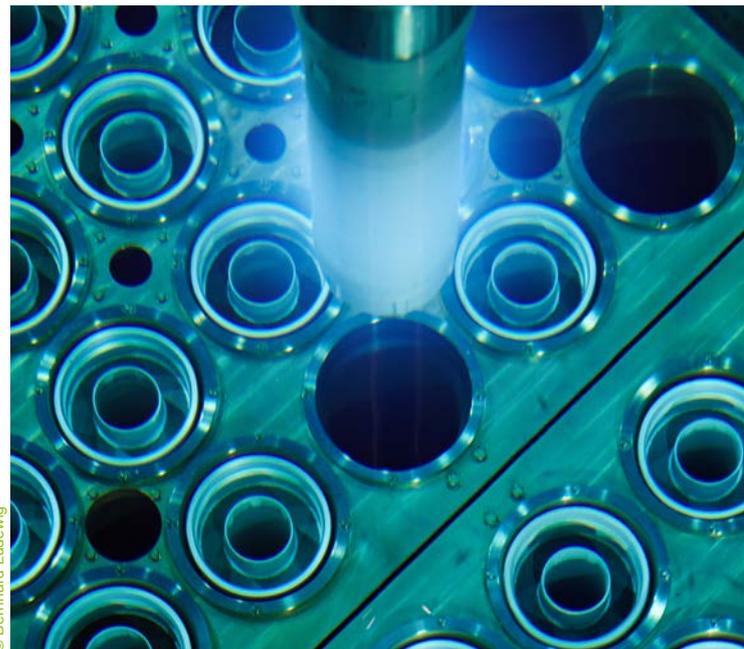
3. Rolling/Plate inspection: In the dispersion process, the fuel core, frame and cover plates are joined together in a solid metallic composite by hot rolling – an inspection afterwards guarantees that everything is perfect.
4. Assembly: Then, the fuel plates are assembled by welding and swedging into a notched aluminium structure that forms the fuel element.
5. Assembly inspection: Finally, the assemblies go through complete inspection controls to ensure a high quality product.

Transport to Garching

The fresh fuel elements are transported by road with a highly secured special transport vehicle in accordance with the transport licenses of both the French authorities and the Federal Office for the Safety of Nuclear Waste Management (BfE) from their production plant in France to Garching.

Operation and use

The FRM II is a heavy water moderated and light water cooled research reactor exhibiting a thermal power of 20 MW. For a cycle of 60 days (1200 MWd), one single cylindrical fuel element is used. The goal is a high neutron flux of $\sim 8 \cdot 10^{14} \text{ n/cm}^2\text{s}^{-1}$.



© Bernhard Ludewig

Fig. 2: Wet storage at FRM II.



Fig. 3:
CASTOR® MTR3/
GNS.

fuel elements. It mainly consists of a ductile cast iron cask body, a fuel basket and a double lid system with metallic sealings. The CASTOR® MTR3 is 160 cm high and weighs 16 t. It was tested by the Federal Institute for Materials Research (BAM) and Testing and approved by the BfE in January 2019.

Transport to Ahaus

For transport, a cask with five fuel elements is loaded onto a special transport vehicle and driven to Ahaus, a town in western Germany near the Dutch border. It consists of a tractor and a semi-trailer combination that are designed in accordance with the "Directive for protection against disturbance measures or other effects by third parties during the transport of nuclear fuels by road and rail" (SEWD Richtlinie of BMU).

Interim storage

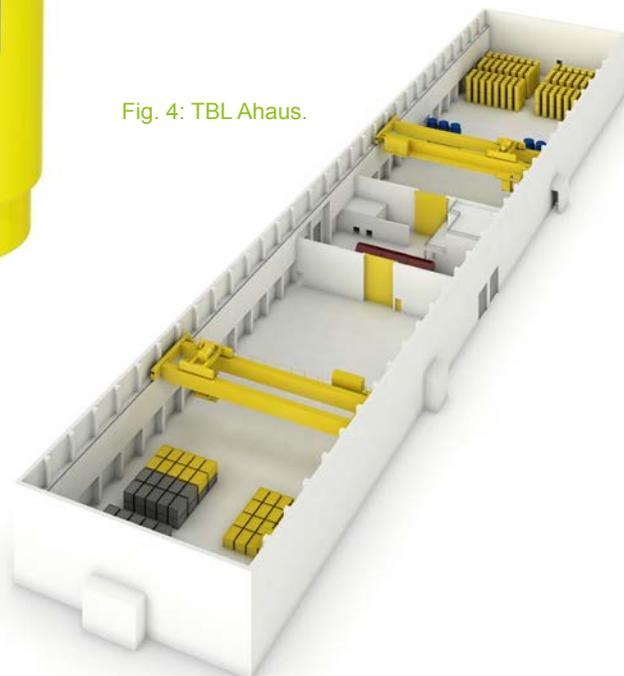
The Transport Cask Storage Facility (TBL) Ahaus is operated by the federally owned Gesellschaft für Zwischenlagerung mbH (BGZ) and the central facility in Germany intended for the interim storage of research reactor fuel elements. The current storage capacity for spent fuel elements of the FRM II in Ahaus extends over seven storage locations for 21 casks. This results in a total capacity of 105 spent fuel elements because three casks can be stacked on top of each other.

Final disposal

A repository still has to be found in Germany. Whether and to what extent further conditioning of the fuel elements is necessary before they are placed in that future repository depends on the storage conditions there.

A. Görg (FRM II)

Fig. 4: TBL Ahaus.



Storage pool

At the end of the cycle, the spent fuel element is unloaded and then transported under water (natural shielding against radiation) to the wet storage of the FRM II where it decays for a minimum of 6.5 years (see fig. 2).

A total of approx. 6.9 kg U are then contained in the spent fuel element of which approx. 6 kg are still ^{235}U . Thus, its enrichment is approx. 88 % of the ^{235}U and the gross mass amounts to about 44 kg (after cutting off the metallic head). The maximum activity inventory is approx. $8 \cdot 10^{14}$ Bq whereas the maximum residual heat (thermal power) is approx. 55 Watt. All figures refer to the end of the above mentioned minimum decay time before a transport is possible.

Transport and storage cask CASTOR® MTR3

The transport and storage casks must withstand thermal and mechanical loads, shield the radioactive inventory safely and dissipate the heat emanating from the radioactive inventory. The CASTOR® MTR3 (see fig. 3) cask, newly designed for this purpose in accordance with the safety standards of the International Atomic Energy Agency (IAEA), contains five FRM II

Tobias Chemnitz

I'll be the new instrument scientist of MEDAPP starting on June 01st, 2019.

I am currently finishing my PhD here at th MLZ about the "Development of a dry-chemical process for the separation of Mo-99 from U-235 targets". This project is performed in close collaboration with Florian Kraus, an expert in fluorine chemistry at the Philipps-University in Marburg.

Due to my work in Marburg I became especially interested in the fluorine chemistry of uranium and its fission products. Furthermore, I'm interested in medical physics, where I'm currently getting an additional master's degree at the Distant and Independent Studies Center at the TU Kaiserslautern.

tobias.chemnitz@frm2.tum.de

at MEDAPP

Newly arrived

Francesco Guatieri

I am the new instrument scientist of the NEPOMUC beamline at the MLZ.

I obtained my PhD working on positronium production, manipulation and spectroscopy at the positron laboratory of the university of Trento and at the AEGIS experiment at CERN. I performed experimental measurements and developed techniques to simulate the behavior of positronium atoms inside of nanochanneled silica.

My special interests are positron and positronium physics as well as antimatter manipulation. On top of that, numerical techniques for the operation, read-out and simulation of antimatter-related experiments.

francesco.guatieri@frm2.tum.de

at NEPOMUC

at the MLZ!

Christian Lang



I joined the MLZ as postdoc and instrument scientist on KWS-2, after my PhD with the topic of non-ideal liquid crystals which I investigated with rheo-SANS and HDLS.

My research interest is soft matter with an emphasis on bio-macromolecules and their structural development in and out of equilibrium. For this purpose, I will implement an in-situ size exclusion chromatography option.

I also plan on expanding the existing rheological tools at the instrument by a shear cell, to investigate the macromolecular ordering in the flow-gradient plane, and a capillary breakup extensional rheometer.

c.lang@fz-juelich.de

at KWS-2

Xiaosong Li



In the beginning of this year I came back to the MLZ from the Radiochemie München (Institute for Radiochemistry), where I worked in the field of neutron activation analysis and gamma spectrometry in the last six years. I join the PGAA-group as an instrument scientist and continue my work at the MLZ right now.

Actually, I am not really a “new-comer” here! After my PhD at the old reactor FRM, I joined the reactor staff and took part in the commissioning process of the FRM II.

I was deputy head of the irradiation division at FRM II and involved in many projects, above all, the silicon doping system and the gamma irradiation device.

xiaosong.li@frm2.tum.de

at PGAA

Newly arrived at the MLZ!

Adrian Losko



I am the instrument scientist for NECTAR and in this position I will support the user programme and develop new imaging capabilities.

I earned a Ph.D. in physics, developing quantitative imaging using the pulsed neutrons at the Los Alamos Neutron Science Center to provide unique characterisation capabilities for advanced neutron imaging and diffraction for next generation fuel characterisation.

My research interest is in utilising particle physics to build new 2D-detectors with application to neutron radiography and tomography.

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at NECTAR

Heiko Saul



I am a postdoc at the new MEPHISTO beamline for fundamental physics which will be set up in the new Neutron Guide Hall East.

I already spent some time at the MLZ during my PhD in which I dealt with the analysis of neutron beta decay studies.

As particle physicist I am interested in the decay process of the neutron. My main interests are the nature of the weak interaction and the search for physics beyond the standard model. I will join the team that sets up and runs the new neutron decay spectrometer PERC at the MEPHISTO beamline. Here we will perform beta decay measurements with improved sensitivity.

heiko.saul@frm2.tum.de

at MEPHISTO

MLZ User Meeting

Garching
Dec. 10th-11th, 2019



How can the MLZ User Committee help you?



The MLZ User Committee meeting in Garching in January 2019.

User Committee members

Adrian Rennie (Chair)

Uppsala, Sweden
adrian.ennie@physics.uu.se

Sophie Combet (Deputy Chair)

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Rainer Niewa (KFN Observer)

Stuttgart, Germany
rainer.niewa@iac.uni-stuttgart.de

The difficulties in transport of fuel have had major impact on the operation of the FRM II reactor and the availability of the facilities for neutron scattering and other experiments. Obviously, this has disrupted plans of many users. Apart from the request for information about a revised operation schedule, this problem gives rise frequently to a follow-up question asking what can be done to improve the situation. Apart from recognising and supporting the efforts of the MLZ management, it is important that, as users, we all state clearly the essential need for these facilities to support work that tackles many important societal challenges. Information about this requirement for advanced research facilities must be spread widely, and not just amongst colleagues and specialists. All of us must help with this task to promote wide support. We can help each other with this duty by sharing information about good examples of success from relevant experiments.

The User Committee for MLZ has been working for slightly more than a year. It has met twice with the MLZ directors for face-to-face discussions on issues that have been raised. Regular teleconference meetings occur between these discussions. Frequently, even if problems have arisen there is a comment that staff at MLZ have been very helpful in minimising the impact. It is important to record both plaudits and suggestions for improvements. Information is passed-on without disclosing individual names.

Ideas from the user community have been received in various ways. There are e-mail messages, contact at conferences and workshops as well as discussions with individual users when members of the committee are present in Garching. Please feel free to tell any of us your views and ideas. We also look forward to seeing you at the User Meeting in December.

A. Rennie (Uppsala University)

Next Proposal Deadline: September 13th, 2019

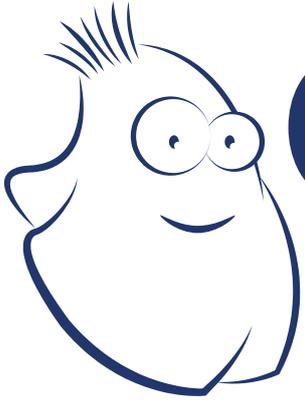


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Next Rapid Access Deadline: July 05th, 2019



Get a first glimpse!



GhOST

Garching Online System Tool

We are proudly announcing the start of our new User Office Online System GhOST in 2019! We worked on it quite some time together with an external company and are getting really thrilled to share the newborn with you in the next future!

It's full name is **Garching Online System Tool** and it helps you with all things related to your beam time here at Garching:

- submit your proposals
- receive and answer questions during the review process
- find the results of the review
- enter your preferred and blackout dates for your experiment
- create your experimental team
- apply for your visit
- submit your experimental report



We will start step by step with the new system. That means, first you will be able to create an account and submit a proposal there – but will still apply for a visit in this year's last cycle via our old system.

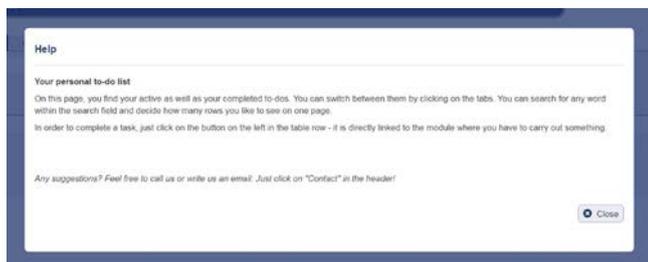
Unfortunately it is not possible to migrate accounts between both systems – this is not only due to technical reasons but also due to statutes (maybe you remember all the problems in the scope of the new GDPR last year...). That means, we will have to ask you to create a new account. But don't worry, this will only take a moment and then you are part of GhOST!

On the right you can see the usual start page of our current User Office Online System. This system has accompanied us – and all our users – since the beginning of user operation here at Garching!

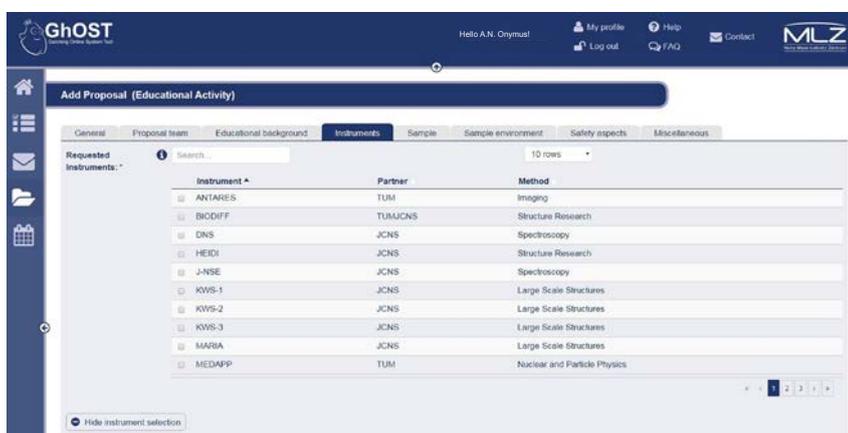
On the left you can get a first glimpse at the new start page. It is looking beautiful, isn't it?

The new sidebar offers you from top to bottom access to the start page, your to-do lists, your messages, your proposals, and your experiments.





There are two possibilities to get help: Each page has a detailed description you can access by clicking on the HELP-button in the header (left). Each field in a form has also a quick info – just move your mouse over the “i” (right). Ups – and a third option: Just call the User Office!



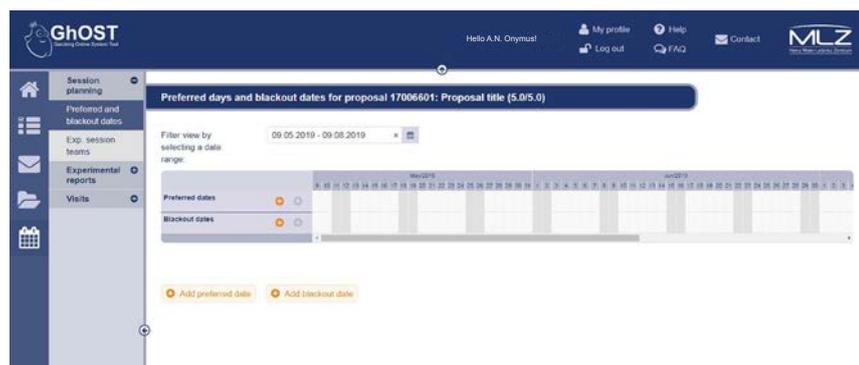
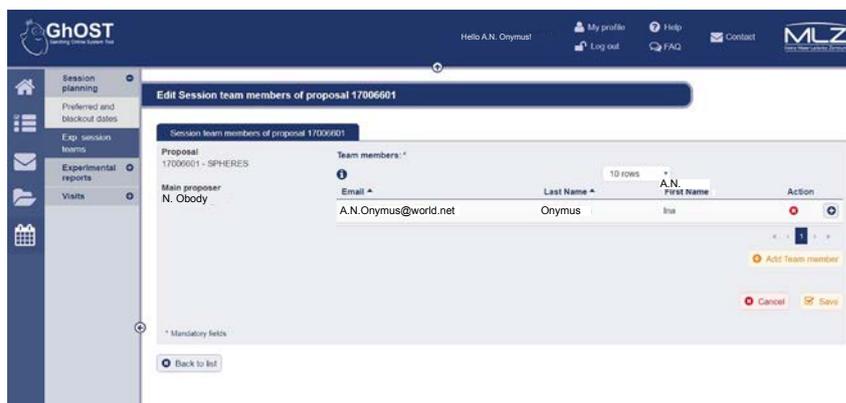
This is a feature many users asked for: Submit ONE proposal and ask for beam time at SEVERAL instruments at the same time!

With GhOST, this is possible. The system creates the other proposals automatically from your input in the main proposal.



In GhOST, each experimental session has a special team. This has to be created before the visit starts – only team members will be able to apply for the visit

This is great because the members can be reminded before the application deadline of three weeks: Thus, we can guarantee your smooth access to the instrument!



Another really cool feature is this table of preferred and blackout dates.

After your proposal was accepted, you are asked to complete this table in order to simplify the planning of the experiment according to your wishes



UPCOMING

MLZ Conference 2019: Neutrons for information and quantum technology

June 04th- 07th, Lenggries (Germany)

<https://indico.frm2.tum.de/e/nfiquat>

ECNS 2019

European Conference on Neutron Scattering

July 01st- 05th, St. Petersburg (Russia)

<http://ecns2019.com/>

Visit our booth there!

School: Neutrons for membrane biophysics

July 15th- 19th, Garching (Germany)

www.fz-juelich.de/jcns/SINE2020

23rd JCNS Laboratory Course – Neutron Scattering 2019

September 02nd-13th, Jülich + Garching (Germany)

www.neutronlab.de

JCNS Workshop 2019 – Trends and Perspectives in Neutron Instrumentation: Probing Structure and Dynamics in Soft Matter

October 07th- 10th, Tutzing (Germany)

www.fz-juelich.de/jcns/JCNS-Workshop2019

MLZ User Meeting 2019

December 10th- 11th, Garching (Germany)

<https://indico.frm2.tum.de/event/171/>

Reactor Cycles 2019

No.	Start	Stop
46b	05.02.2019	11.03.2019
48	16.07.2019	13.09.2019

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Mirror, mirror on the wall...

Photo taken by Dr. Karl-Heinz Rothenberger.

Wasser!

