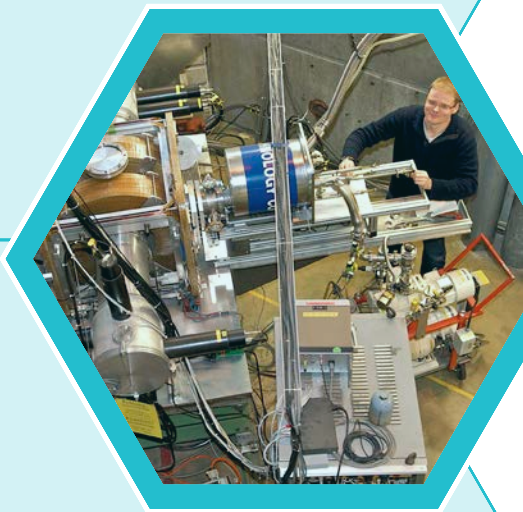
- NMI3: a success story -

Neutrons and Muons for Europe 2009-2013



nmi3

SEVENTH FRAMEWORK PROGRAMME

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Editorial

With the completion of a second European contract in January 2013 the integrated infrastructure initiative NMI3 has reached a further milestone.

The moment is, therefore, adequate to take stock. In order to avoid a view tinted by rose-coloured glasses, the exercise is best left to an outside body like the NMI3's independent Advisory Committee (AC). After having participated for two full days in the discussions of the final General Assembly (Technical University of Munich, December 5-6, 2012), Romano Rinaldi as AC chairman summarised the assessment as follows:

"In this day and age, when the European Union seems to be hit by some critical challenges as to its own integrity, it is quite reassuring to assess the results obtained by NMI3. Although representing a relatively small enterprise, the activities of the research groups involved provide a good example of work in the direction of a true European integration worth its name (as indeed the acronym NMI3 is calling for). This is even more so when considering the great achievements obtained in terms of absolute scientific value as well as in terms of cost effectiveness. NMI3 is an example of both collaborative effort and healthy competition among scientists and institutions belonging to many different countries of the Union; often seen redundant at a first superficial glance and here proving what results can be achieved once their effective complementarity is put to work for the benefit of the entire community".

This achievement is certainly something that all the actors within NMI3 can be enormously proud of. NMI3 has delivered on all fronts more than could reasonably be hoped for. Despite its short duration of only 2 years, the Transnational Access Program produced exciting experimental results. The work of the Joint Research Activities was not only of utmost scientific relevance but fed quickly into the experimental facilities thus helping to provide better service for the users. Education and dissemination within NMI3 have become a reference way outside Europe.

However, what probably has to be considered the greatest achievement of NMI3 is its ability to create an intense nearly family-like climate of collaboration. I am convinced that this climate motivates people to perform at the highest possible level. It has been an immense pleasure to be part of this exceptional family as coordinator for the past four years. I am deeply indebted to the whole NMI3 for having made my task so easy and so enjoyable. I wish NMI3 all the best for the future and I am fully convinced that the best for NMI3 is still lying ahead.

Helmut Schober
NMI3-I coordinator

NMI3 supports European neutron and muon research through:

Joint Research Activities

The Joint Research Activities (JRAs) supported by NMI3-I have brought experts together from facilities across Europe to develop new techniques and instrumentation for neutron and muon research. In the following interviews and articles the coordinators of the six JRAs supported by NMI3-I look back on the experience and their JRAs‘ achievements.

Access Programme

NMI3 provides support for neutron and muon scientists to access the best of 8 facilities’ instruments across Europe. The results of this research have implications in fields as varied as medicine or agriculture, the arts, transport, and information technology. This brochure contains research highlights from our Access Programme during the NMI3-I funding period.

Networking Activities

With its networking Activities, NMI3 supports trans-facility collaborations aiming to improve the experience of European scientists using neutron and muon beams, provides funding to schools that address a broad range of topics, and increases the visibility of the work of neutron and muon researchers across Europe.

Neutron and muon research through NMI3-II

NMI3-II continues to support European neutron and muon facilities. Previous Joint Research Activities (JRAs) will extend their research work through NMI3-II. For instance, the Muons JRA, coordinated by Stephen Cottrell from ISIS, will continue to develop technologies and techniques to extend the range of capabilities of the muon method available to European users. Nigel Rhodes from ISIS is now the coordinator of the Detectors JRA, taking over Karl Zeitelhack from FRMII. The work of this JRA focuses on the development of two promising detector technologies.

New collaborations are also ongoing. Nikolay Kardjilov from the Helmholtz Zentrum Berlin coordinates the Imaging JRA on the development of new methods and tools that will allow to probe micro and nano structural properties of composite materials using imaging in real and reciprocal space. Annie Brulet from the Laboratoire Léon Brillouin is the coordinator of the JRA on Advanced Neutron Tools for Soft and Bio-Materials, which aims to provide a wider range of experimental tools enabling the best use of neutron scattering for soft and bio-materials.

Furthermore, as a result of the NMI3-I Monte Carlo and Data Analysis collaborations, in NMI3-II the ‘Data Analysis Standards’ project will focus on improving software for data analysis, to help users deal with the ever-increasing amounts of data and speed at which experiments are carried out.

Joint Research Activities

The Muon JRA – new technology for the future of muon research

Partners:

University of Parma, Italy

University of Babes-Bolyai, Romania

Paul Scherrer Institut (PSI) Continuous Muon Facility, Switzerland

ISIS Pulsed Muon Facility, UK

Coordinator: Stephen Cottrell, instrument scientist at ISIS

How did the idea for this collaboration come up?

The collaboration between the facilities arose naturally from a common requirement for new technologies for high field μSR. At the time, each facility was developing a new high field spectrometer and coming up against similar technical problems. Therefore, it was natural for us to work together to find solutions to mutual problems; development of instrument simulation codes and new types of detectors came from this collaboration. Meanwhile, a number of university groups had ideas for developing technically challenging μSR techniques, such as pressure measurements or RF methods, and the JRA was an ideal way for them to collaborate with facility scientists on these developments.

What was it like coordinating collaboration between the different members of the JRA?

The collaborations within the JRA have worked well, with activities focussed by a common theme. Work was coordinated by looking well ahead to remind groups of forthcoming milestones and deliverables. Regular meetings gave us a chance to catch up on what everyone was doing and also provided the opportunity to discuss any issues arising with the projects. In fact, one of our biggest problems came from the fluctuating exchange rate: this affected the amount of money available to spend on the project at a given time – but this was outside our control!

What have you and the others involved learned from this collaboration?

The benefits of being involved in the collaboration are huge! Individually, the facilities are working to solve specific problems that optimise the performance of new instruments, while University groups help drive the innovation of new experimental techniques in order to solve their immediate scientific problems. By working together, supported by funding from the NMI3, we've found we can achieve much more. For example, we've been able to provide general tools for tackling problems such as instrument design and detector development, while new experimental methods have been demonstrated and then made available to the wider scientific community.

What are the advantages of taking part in a project supported by NMI3?

The support from NMI3 has been absolutely crucial to the various collaborations included in our JRA. It's provided funding for equipment and, most importantly, staff; giving us the resources to develop and test new techniques that have been used for the new high field spectrometers and novel experiments. Funding for travel has also been important, as it's allowed us to get together to discuss our projects and present our work at international meetings – this is really important for making people aware of what's possible with μSR. It's also good to be part of a wider collaboration; the General Assemblies are a useful forum for meeting and exchanging ideas with others working in similar areas.

What are the plans for your future research? Will you continue participating in this type of collaboration?

The muon community certainly hopes to continue participating in this type of collaboration – we have lots of good ideas for developing aspects of the μSR technique that we're keen to take forward! In the next contract (NMI3-II) we'll continue with the theme of high field μSR, with work focussing on improving codes for data analysis and engaging in outreach to make the wider scientific community aware of these new techniques. Looking to the future, there are quite a number of groups keen to work together to develop DFT codes both for calculating hyperfine couplings and predicting the muon site in materials, and then there are ideas for new, intense muon sources that we want to look into.

Europe is fortunate in having two muon sources that are complementary and together offer researchers access to the full range of muon spectroscopic methods. The Muon Spin Resonance (µSR) technique is remarkably versatile, encompassing studies of magnetism, superconductivity and spin and charge transport, while providing a highly sensitive hydrogen analogue to probe semiconductors and proton conductors. The technique has an important role beyond condensed matter physics, and offers chemists a valuable method for investigating the fundamentals of reaction kinetics. It is also an excellent tool for the study of organic radical structure and dynamics in solids, liquids and gases. The beam structure of the SµS, located at PSI, makes it ideally suited for applications where high timing resolution is essential to follow fast muon precession or rapid spin depolarisation. In contrast, the pulsed nature of the ISIS beam, operated by the Science and Technology Facilities Council in the UK, allows low background time differential data to be captured at high data rates, while enabling the effect of beam synchronous excitations (such as Radio Frequency or laser radiation) to be easily investigated. The work of the JRA in Muons has stimulated development of a broad range of source technologies, while engaging the user community to research novel experimental techniques and analysis tools. Together, this work is now making a significant impact on European muon research.

Developing µSR in high magnetic fields

The development of new instruments for high magnetic field spectroscopy was essential to provide the user community with the tools necessary for future research. However, µSR in high magnetic fields is uniquely challenging. Both the implanted muons and detected decay positrons are charged and their trajectories are modified by the applied field. The detector systems need to be field insensitive yet capable of providing fast-timing. A significant aim of the JRA has been to develop the technologies required for high field µSR spectroscopy. The importance and success of this work is evidenced by recent grant awards to both facilities to develop high field instruments. The ISIS instrument (fig 1, top) provides a 5T field parallel to the muon spin polarisation and offers a sample environment covering temperatures between 25mK and 1200K. The instrument is now fully integrated into the ISIS user programme and has already been used for a broad range of studies, with journal publications in frustrated magnetism, molecular nanomagnetism and molecular radicals. In contrast, the spectrometer at the SµS (fig 1, bottom) is optimised for measurements whe-

Fig 1. ISIS high field spectrometer (top) and the high field spectrometer at SµS

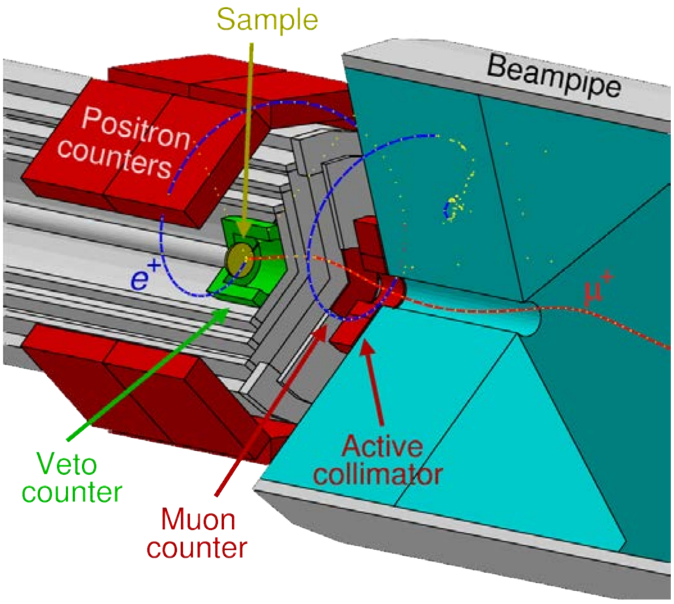


Fig 2. A study of the detector geometry and positron trajectories for the SμS high transverse field spectrometer

re the 9.5T field is perpendicular to the spin polarisation. Test experiments have confirmed excellent performance through the measurement of full amplitude spin precession signals at approximately 1.29GHz in the 9.5T field. Fast timing at sample temperatures below 20mK has been achieved through the development of a novel optical readout for the dilution fridge. The instrument is currently being commissioned in preparation for user experiments.

Simulation codes and beam diagnostics to characterise muon and positron profiles

A comprehensive suite of simulation codes was developed to model both the profile of the muon beam through the instrument and the positron track to the detector. The program, musrSIM, based on the popular Geant4 toolkit, enables the instrument geometry, materials and field profile to be defined. It also allows us to study the response to muons and decay positrons. Input can be taken from beam simulation programs to accurately model the incident muon beam, while the response can be analysed and tested for various acquisition parameters using the associated application musrSimAna. The codes played a crucial role in the development of the detector arrays for both the ISIS and PSI instruments. As an example, figure 2 shows a study of the detector geometry used for the SμS spectrometer, and illustrates the need to consider positron spiralling when locating the positron counters.

We checked our early simulation results during experimental work at the SμS, making use of a novel position-sensitive scintillating fibre detector developed within the JRA for profiling muon beams in high magnetic fields. Detailed beam profiles were obtained using a grid of 20 fibres covering an area of 10x10cm^2, with a readout using avalanche microchannel photodiodes enabling a compact design and assuring insensitivity to magnetic fields. The development of the ISIS high field instrument required new technologies for direct imaging of muons, since we needed a detailed understanding of how the muon spot evolved in position and shape in the applied field at the sample position. We achieved this by developing a field-insensitive beam camera, using a high sensitivity cooled charged-coupled device (CCD) to image the light from a scintillating screen mounted on the sample stage of the cryostat. The device proved crucial to the commissioning of the spectrometer, enabling the muon spot to be monitored as automatic systems were developed to control and stabilise the beam position with the magnetic field.

Detector optimisation

Significant work was carried out to optimise the detector arrays for high magnetic field measurements. For the ISIS instrument, although the scintillation detectors were, by necessity, positioned close to the sample, we successfully used extended light guides to move the field-sensitive photomultiplier tubes to a low field region. In contrast, the geometry and fast-timing requirements of the SμS spectrometer required a particularly compact detector array. We therefore had to develop a novel detector array based on Geiger-mode avalanche photodiodes (APD) for this instrument. We tested a prototype detector

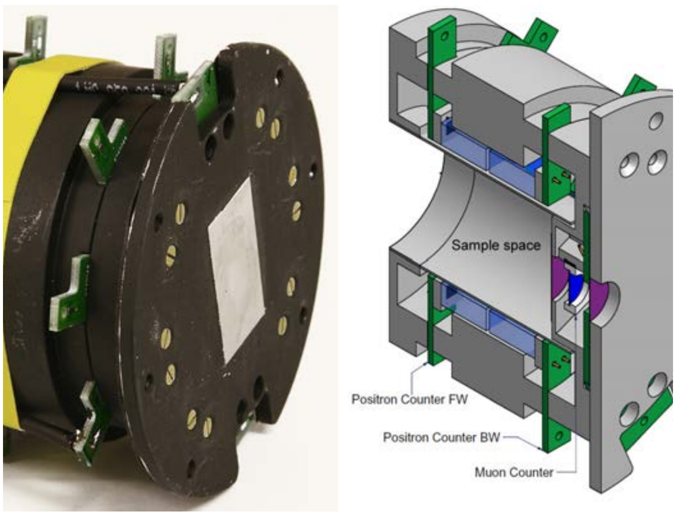


Fig 3. A prototype detector module based on avalanche photodiodes developed at the SμS (left) and schematic view

module (shown in fig 3) to 9.5T at the SμS and obtained excellent results. The measured time resolution was better than 80ps and, most importantly, was shown to be insensitive to magnetic fields.

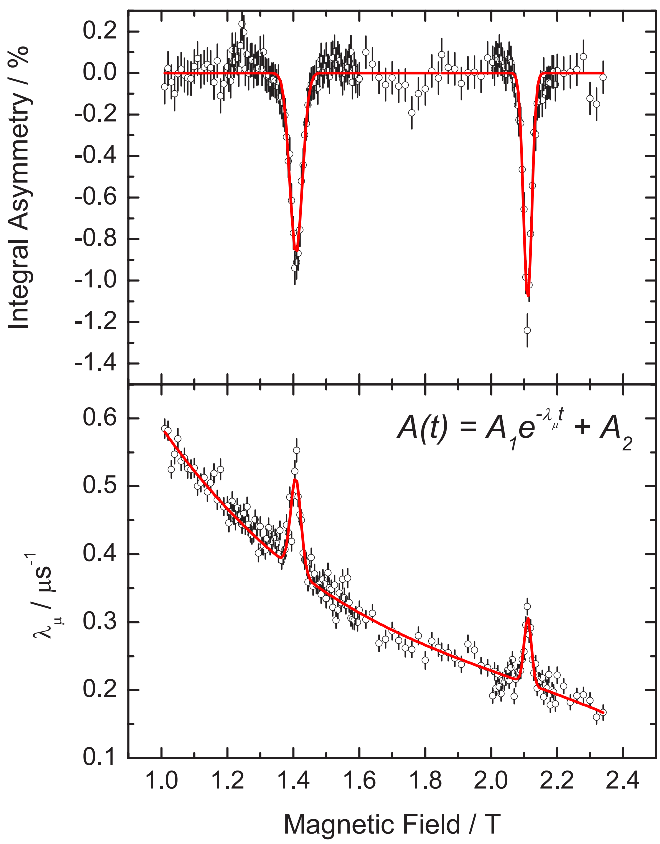


Fig 4: Gas target pressure cell designed for the ISIS high field spectrometer (top) and an avoided level crossing measurement of the Mu-ethyl radical formed by implanting muons in ethene gas at 300K.

Novel resonance techniques for new measurements

Novel NMR-style (nuclear magnetic resonance) pulsed radio frequency (RF) resonance techniques were explored as a means of obtaining new information from μSR experiments. Working in collaboration with a group at the University of East Anglia, two sequences were demonstrated during the project. Firstly, we investigated a double resonance method where both muon and nuclear spins are simultaneously irradiated to decouple the nuclear dipolar interaction. The technique is able to provide unique information about the muon site and dynamics in a system under study. Secondly, we explored a composite spin inversion sequence with the aim of improving the efficiency of RF spin rotation in RF μSR experiments. The pulsed nature of the ISIS beam was crucial to the success of both techniques – the RF excitation can be synchronised to the intense muon pulse, simplifying the setup of complex sequences and avoiding problems associated with RF heating. This work highlighted the need for good RF engineering of cavities to ensure reliable application of suitably intense RF pulses. To this end, we developed both an NMR system to enable off-line tests of RF cavities and a dedicated high power RF insert for the ISIS high field spectrometer.

μSR under Pressure!

Pressure is an important parameter in the investigation of the phase diagram of condensed matter systems and its study can often reveal new and sometimes exotic physical properties of materials. In the gas phase, compared to other resonance techniques, μSR provides a uniquely sensitive tool both for studies that can reveal spectroscopic information and enable a direct measurement of chemical reaction kinetics. An important activity supported by the JRA was the development of sample environment suitable for μSR measurements at high pressures in both the solid and gas phases. Work within this task was led by the group at Babes-Bolyai University and focussed on solving problems unique to μSR. For the solid sample pressure cells we investigated a number of designs with the aim of providing a reliable working pressure in excess of 2.5GPa even at cryogenic temperatures. The cells were configured to use the high energy muon beam available at PSI, and work was carried out to optimise the muon stopping range and maximise the sample signal. The provision of gas target pressure cells for the high field spectrometer was the focus of our work at ISIS, and we recently explored the spectroscopy of small gas molecules during commissioning experiments at the facility (fig 4). We continued this work by commissioning an integral RF cavity to

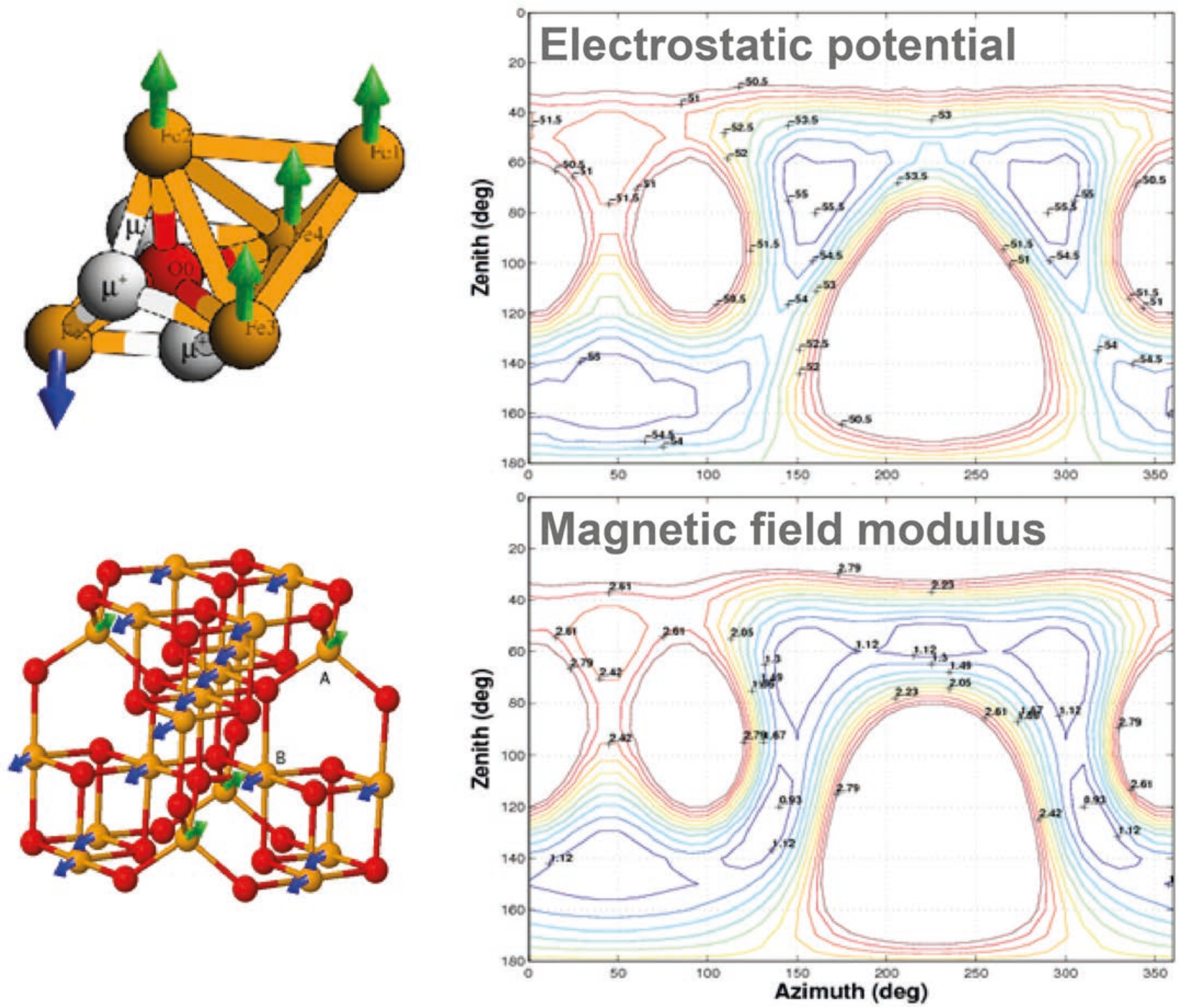


Fig 5: Visualisation of a structure and magnetic moment (left) and a search for muon sites by mapping electrostatic potentials and magnetic dipolar fields.

enable RF techniques to be developed in the gas phase. The system is currently being used in collaboration with a group from University of British Columbia to investigate chemical reaction kinetics for simple abstraction reactions.

New software for data analysis

We have explored new software methods both to support the analysis of complex experiments and to help the community share data and software between facilities. Led by a team from the University of Parma, we developed code to calculate electrostatic potentials and magnetic dipolar fields within magnetic materials (fig 5). Experimental data can be compared to simulation results to help assign muon sites. Work continued to evaluate the potential for using Density Functional Theory (DFT) simulations to establish muon interstitial sites, and it was concluded that an *ab initio* strategy may provide a powerful solution provided the computational complexity can be solved. The development of the NeXus data format provides a basis for storing muon data with comprehensive metadata to properly describe the experiment, a facility that will become increasingly important with the move to open access journals and data repositories. We carried out work to finalise a NeXus

Instrument Definition suitable for both ISIS and PSI, while agreeing an essential subset of data and metadata for use by the worldwide muon community as a Common Exchange Format. This agreement should be beneficial to users as they move between facilities, and make it easier for the facilities and user groups to share software development effort.

Conclusions and future work

For the two European muon sources the work of this JRA has made a significant impact on the instrument suite available to their communities. Activities during both Framework Programme 6 (FP6) and the present JRA underpinned these projects through the development of technologies, such as field insensitive fast-timing detectors and simulation codes, essential for high field μSR. For the scientific community, work within the JRA has provided new equipment and methods for novel experiments that greatly extend the capability of μSR. Importantly, the JRA has given a focus to all these activities, providing resources for groups to work collaboratively to develop high quality long term solutions.

Looking to the future, during our second project under FP7 we are planning to transfer APD detector technology from PSI to ISIS, evaluating its suitability for use at a pulsed muon source. The on-going theme of high field μSR will continue, with work now focussing on the development of efficient algorithms for the analysis of high field experiments. We are also engaging in outreach through workshops, leaflets and websites, with the aim of bring the unique potential of high field μSR spectroscopy to the attention of the wider scientific community.

Recent Publications

Lord *et al.*., *Rev. Sci. Inst.*, 2011
Baker *et al.*, *J. Phys.*, 2011
Lancaster *et al.*, *J. Phys.: Condens. Matter*, 2011
Cox *et al.*, *J. Phys.: Condens. Matter*, 2011
Sedlak *et al.*, *Physics Procedia*, 2012
Stoykov *et al.*, *Physics Procedia*, 2012
Clayden *et al.*, *J. Mag. Res.*, 2012
Prando *et al.*, *Phys. Rev. B* 87, 2013
Cottrell *et al.*, *Physics Procedia*, 2012

Detectors - Grand challenges for neutron detection

Partners:

Institut Laue-Langevin (ILL), France

Laboratory of Instrumentation and Experimental Particle Physics (LIP), Portugal

Science and Technology Facilities Council (STFC), UK

Jülich Research Centre (FZJ), Technical University of Munich (TUM), Germany

National Research Council (CNR), Italy

Coordinator: Karl Zeitelhack, head of the Detector laboratory at FRM II

How did the idea for this JRA collaboration come up?

The idea for this JRA is based on the studies of Gaseous Scintillation Proportional Counters, which have been performed already within the framework of the MILAND Detector JRA during the Framework Programme 6 phase of funding. Given that very interesting and promising results could be achieved in these studies, we found it very attractive to further investigate on this.

What was it like coordinating collaboration between the different members of the JRA?

This JRA was particular simple to coordinate as almost all partners had good relationships and bilateral collaboration before.

What have you and the others involved learned from this collaboration?

The work performed within this JRA has given a deep insight in the physical processes and technical aspects underlying the technique of a Gaseous Scintillation Proportional Counter. We have certainly acquired significant knowledge on the performance of this type of detector, its benefits and its limitations.

What are the advantages of taking part in a project supported by NMI3?

This type of project pursued in an international collaboration allows the study of new arising technologies that cannot be used yet in a detector for a real instrument.

What are the plans for your future research? Will you continue participating in this type of collaboration?

Yes, we certainly will. Most of the partners participating in this JRA are members of the new detector JRA or are engaged in similar collaborations.

In view of the upcoming new generation of powerful spallation sources, the benefit of a higher neutron flux relies on the development of new, fast and highly efficient neutron detection systems. From a physical point of view, the detection is based on the absorption of the neutron and the subsequent recording of either the electrical charge generated or the light emitted through the absorption process. The best performance so far has been achieved using ^{3}He gas as absorbing material, both in terms of detection efficiency and an optimal signal-to-noise ratio. On the other hand, scintillation counters based on solid converters such as Li-glass, which detect the emitted light, are capable of faster detection: they can record more neutrons per detection area and achieve a better time resolution if required.

Six European partners have teamed up in a JRA to develop a detector in which both of the effects described above are combined. In this so-called Gaseous Scintillation Proportional Counter (GSPC), the absorption of the neutron in the nuclear reaction with ^{3}He generates a 'primary' light pulse, and when the charge released in the gas reaches the charge amplifying region of a micro patter device like a MicroStrip Gas Counter (MSGC) it generates a much brighter 'secondary' pulse.

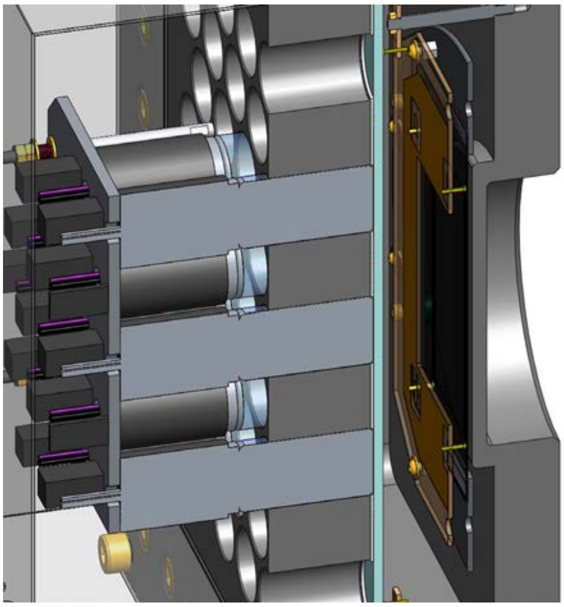
Spatial precision of detection is very important for modern neutron applications. In the GSPC detector, this is achieved by using several detectors of light called Photo Multiplying Tubes (PMT) in a particular array. The main tasks of this JRA project were to investigate this new detection process and develop adequate readout electronics. The aim was to demonstrate the feasibility of this new kind of detector within 20 × 20 cm^2 active area capable of achieving a 0.5mm position resolution together with a count rate capability close to 1 MHz.

Gaseous Scintillation Proportional Counters

MSGC operating with a gas mixture of ^{3}He-CF_4 are very efficient for the production of fast scintillation light with wavelengths between 150nm and 750nm. Spectral response and photon yield are strongly dependent on the CF_4 partial pressure and the electric field applied in the detector.

In precise studies performed at LIP and ILL, we obtained emission spectra of CF_4 fully corrected for spectrometer and PMT sensitivity for various gas pressures. With rising CF_4 pressure the photon yield increases up to ~0.19 photons / secondary electron at 5 bar. Decay times as short as τ ~ 15 ns could be confirmed for both the primary and secondary scintillation light. These values guarantee a dead time shorter than 100 ns per event in a real operational system.

In addition, the performance of a potential GSPC mainly depends on the light readout scheme, as well as optical and geometrical parameters such as photon detection efficiency, readout pixel geometry and position reconstruction. All these parameters have been taken into account in the comprehensive software package ANTS developed at LIP Coimbra. ANTS comprises two modules: a simulation module for evaluating



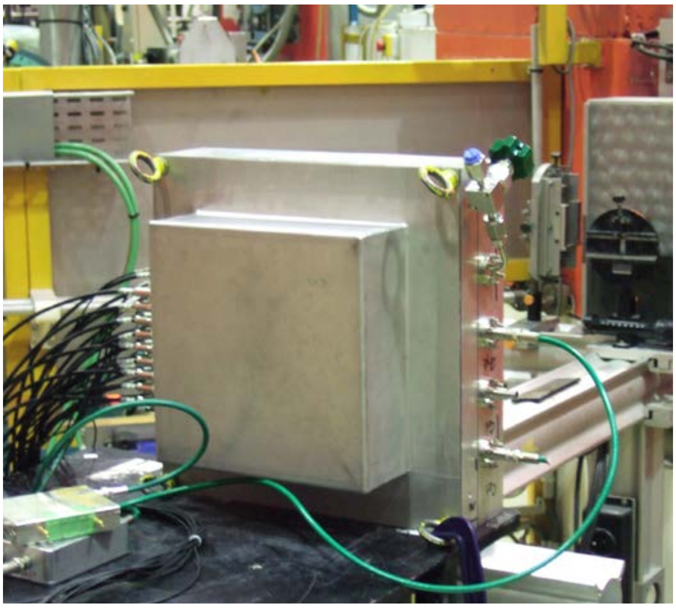


Fig 1. Schematic cross-section of the GSPC prototype developed at ILL and tested on CT2

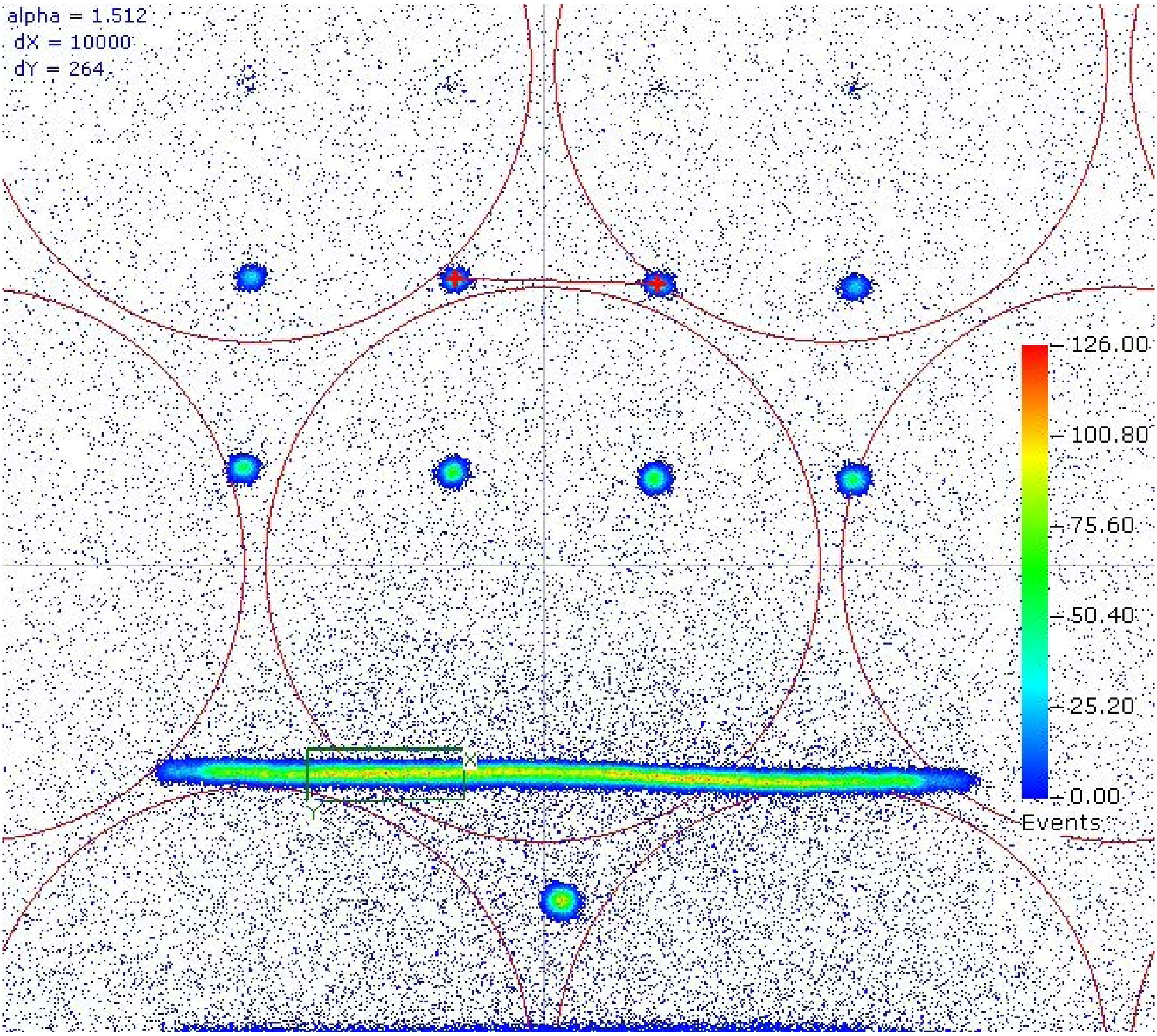


Fig 2. 2D-position spectrum resulting from the neutron beam test with the readout electronics

the performance of different GSPC designs, and an analysis module for processing either simulated or experimental data using sophisticated algorithms for calibration and position recognition.

Light readout devices and electronics

The performance envisaged can only be achieved with the proper light readout device and sophisticated, fast readout electronics, capable of handling high data rates and performing complex position calculation algorithms.

A set of three identical small-size prototype detectors were built at FRM II and distributed to the partners at STFC and FZJ. In a series of complementary studies, the number of detected photoelectrons could be increased using a MSGC developed at ISIS and PMTs with UV window and red extended photo sensitivity. The position resolution was correspondingly improved.

A dedicated 32-channel readout electronics system for an Anger Camera GSPC has been built at FZJ. Its architecture is based on a charge-sensitive preamplifier pulse-shaping stage and an 80 MHz (12bit) sampling ADC for each PMT channel with FPGA-based pulse processing. The self-triggering system allows raw data storage on disk via a GBit optical interface for the development of reconstruction algorithms. Online event reconstruction could be implemented in the FPGA or on a Graphics Processing Unit connected to the readout system.

A different, interesting approach is being followed by the STFC team. By applying a commercially available FPGA-based evaluation board, capable of reading 150 MHz sampling ADCs, the team studied the performance of an on-board implementation of the position recognition software, using a neural-network-type algorithm.

GSPC 19 demonstrator detector

Based on the results achieved during the programme, a large area GSPC demonstrator with Anger Camera readout has been designed and built at ILL. For the first measurements, the detector shown in Fig 1 was filled with a gas mixture of 1 bar Helium-3 and 6 bar CF_4. It is equipped with a 9 cm x 7.3 cm active area MSGC developed at ISIS and an array of 19 Hamamatsu R5070A PMTs for the readout.

In autumn 2012, a first test on the neutron beam with the readout electronics was performed at the CT2 beamline at ILL. Fig 2 shows the resulting 2D-position spectrum recorded with the 32-channel readout system when the detector is homogeneously illuminated with 2.5A neutrons with a multi-hole / slit boron-nitride mask mounted in front. The hole diameter is 0.5 mm on a 10 mm pitch, while the slit width is 0.2 mm. A position resolution of $\Delta x \sim 0.6$ mm (FWHM) close to the physical limit is achieved by analysing the data with ANTv.06 using a maximum likelihood reconstruction.

Conclusion

This JRA has intensively explored the potential of new technology for neutron detection. Lively and very effective collaboration amongst the partners is now sharing expertise on GSPCs and combining the different technologies available in the individual groups. This is reflected in the various joint training schools and experiments that have been performed with participants from all the partners involved. This collaboration is well set to continue developing GSPC detectors in the future.

Recent Publications

Morozov *et al.*, *Nucl. Instrum. Methods*, NIM A 268 / 9, 2010

Morozov *et al.*, *Nucl. Instrum. Methods*, NIM A 628 / 1, 2011

Morozov *et al.*, *J. Instrum.*, JINST 7, 2012

Margato *et al.*, *Nucl. Instrum. Methods*, NIM A 695 /11, 2012

Casinini *et al. Nucl. Instrum. Methods*, NIM A 675, 2012

The Deuteration JRA: novel methods for sample production in biological systems

Partners:

Institut Laue-Langevin (ILL), France

Laboratoire Léon Brillouin (LLB), France

Neutron Research Reactor Heinz Maier-Leibnitz (FRM II), Germany

Max-Planck-Institute for Biochemistry (MPG.IBCHEM), Germany

Rutherford Appleton Laboratory/ Science and Technology Facilities Council (ISIS/ STFC), UK

Coordinator: Trevor Forsyth, instrument scientist at ILL

How did the idea for this JRA collaboration come up?

Macromolecular deuteration and other forms of isotope labelling are major priorities in optimising neutron scattering and NMR studies of biological systems. A strong network of scientists has over the years collaborated on the scientific projects and on the development of new methodological approaches. This led to the formation of the Deuteration JRA, with partners from ILL (Life Sciences group), FRM II (Michael Sattler), ISIS at Rutherford Laboratory (Luke Clifton), IBS Grenoble (Christine Ebel), and MPI Martinsried (Hermann Heuman). The purpose of the JRA was to develop a new range of techniques that would enhance the efficiency and effectiveness of existing work, and also broaden the scope for this area of science in the future.

What was it like coordinating collaboration between the different members of the JRA?

It was a pleasure to work with such talented JRA partners and to see the outcomes of the project deliver such a strong impact - both within the consortium and also to the wider scientific community.

What have you and the others involved learned from this collaboration?

All of the JRA partners have learnt a great deal from the project. Furthermore, it is clear that the various institutions involved – including facility operators such as ILL, ISIS, FRM II – have learnt a great deal from the work. There are now clear trends towards more integrated approaches in structural biology, and the natural synergy that exists for the needs of the neutron scattering and nuclear magnetic resonance (NMR) communities is an important part of this.

What are the advantages of taking part in a project supported by NMI3?

NMI3 has provided an important political framework linking key large-scale European facilities. This has facilitated connectivity between fundamental scientific activity in the Life Sciences and instrumental developments. Input from biophysicists, biochemists, and molecular biologists in defining instrumental needs is now very evident. NMI3 has also helped emphasise something very obvious but something that is somehow easily forgotten: there is no point in building the best instrumentation in the world if you are not prepared to put serious effort into sample preparation.

What are the plans for your future research? Will you continue participating in this type of collaboration?

The NMI3 Deuteration JRA has resulted in a number of key developments. However there remains a great deal to do for method development. Major progress is possible, for example, in the development of labeling for mammalian cell systems, cell-free synthesis, and in a number of key scientific areas such as the study of intrinsically unfolded proteins (IUPs).

Picture: Serge Claisse, ILL

This JRA has developed protocols that are impacting strongly on the scope and quality of biological neutron scattering experiments carried out at central facilities throughout Europe. The need for this is very clear given the increasing trend towards interdisciplinary and integrated approaches for the study of biological systems. Neutron scattering has a unique and important role to play if the right types of sample can be made available. Deuteration is essential to this: the ability to label complex/interacting systems offers approaches that are simply not possible using other methods. This project has contributed to widen the access of neutron scattering methods to biologists throughout the European Union, both by extending the range of problems that can be tackled, and by reducing the cost impact of sample preparations. It exploits an obvious synergy with the nuclear magnetic resonance (NMR) community, which also has important needs for isotope labelling and within which there is increasing use of neutron scattering.

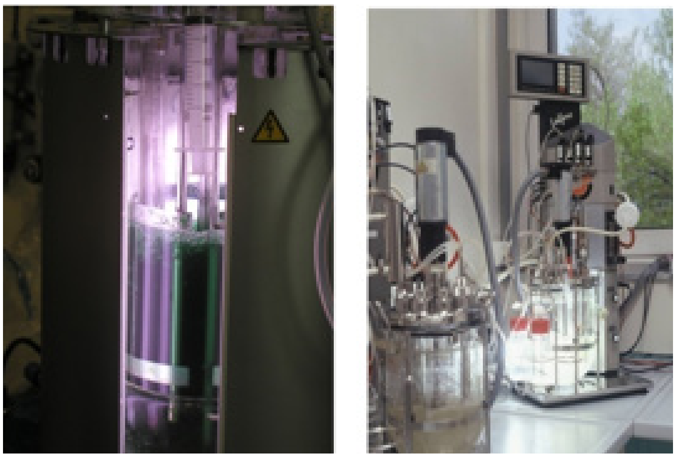


Fig 1. Deuterated biomass production from phototrophic (green algae) and heterotrophic (*E.coli* and *P.pastoris*) micro-organisms

Optimisation of deuterated biomass production

A large number of biological neutron studies rely on the biosynthesis of deuterated biological macromolecules using deuterated carbon sources. The cost of these often limits experiments severely. In this task we have developed protocols for the optimisation of *E. coli* and algal biomass production. Since algae grow photosynthetically, relying only on D_2O medium, CO_2, and light, they are an ideal candidate for cheaper production of deuterated components. Major downstream applications in neutron scattering are obvious for these *in vivo* products: deuterated molecules can be purified and used as deuterated feedstock to bacteria such as *E. coli* and *P. pastoris* (e.g. fig 1).

Production of labelled proteins in yeast

Most proteins used in neutron scattering studies are produced in bacteria such as *E. coli*. This type of protein production has had a huge impact on studies of biological systems using a wide variety of techniques. In many cases the use of *E. coli* is limited by folding/post translational modification problems. Some proteins have to be produced in lower eukaryotic expression systems. However there are difficulties in adapting such cells to growth in deuterated media. Here we have developed methods whereby labelled proteins can be produced (intracellularly or exported) in yeast (fig 2). The successful development of such systems is now opening up completely new areas for neutron-based biomolecular studies.

Segmental labelling of proteins

There is a huge requirement for proteins where extended regions/domains/subunits are selectively deuterated. Development in the method for deuteration now allows contrast matching studies to be carried on a far wider range of sample systems. Over the course of the project we have established two model systems (U2AF65 and TIA-1) for implementing and optimising protein ligation techniques and subsequently demonstrated the expression of fragments and the ligation using protein trans splicing techniques. We have first established the production of segmentally isotope-labeled proteins using segmentally 15N-labeled proteins. We then used the optimised protocol for segmental deuteration of the protein TIA-1 RRM2-RRM3 (fig 3). We have used the purified protein for SANS measurements with contrast variations at ILL Grenoble to document the utility of segmental deuteration.

We have developed a protocol for the production of segmentally deuterated proteins based on the results, which serves as a guideline and recommendation for the neutron community.

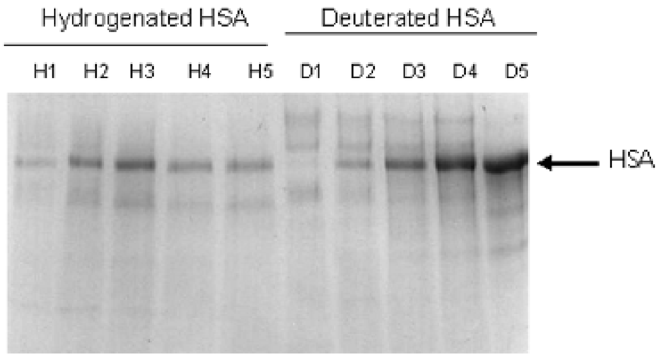


Fig 2: SDS–PAGE analysis showing expression of hydrogenated and perdeuterated HSA in *Pichia Pastoris* cell culture supernatants.

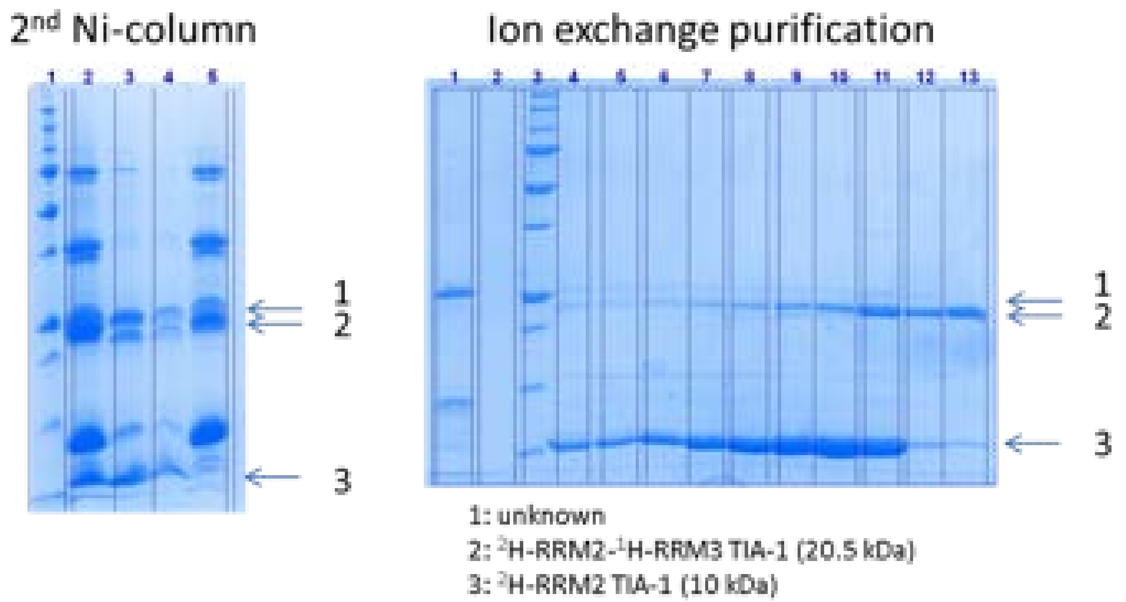


Fig 3: Expression, ligation and purification of a segmentally labeled protein

The experimental protocols and optimisations of the production of segmentally deuterated proteins have been exchanged with the Life Sciences group at the ILL and will thus be available for the general scientific community of neutron researchers. The implementation of the protocol is being prepared for publication.

We have also started to explore the use of sortase-mediated protein ligation, which has been reported to yield better ligation efficiencies compared to intein-based methods. For the TIA-1 model systems, this work is still in progress. However, for another multi-domain protein we have successfully implemented sortase-mediated protein ligation with very high yields.

Low cost D-glycerol production

The high cost of deuterated carbon sources for the expression of D-proteins in *E.coli* is still a stumbling block for the application of neutrons in biology. In this task, we have developed methods for the production of deuterated glycerol by algae under salinic stress. A novel protocol based on "milking" algae of the glycerol produced, dramatically reduces costs because the same biomass and D_2O can be used repeatedly. Approaches have been developed using *Dunaliella salina* and *Chlamydomonas reinhardtii* (a freshwater algae that could be competitive with *Dunaliella*). *Dunaliella* accumulates up to 6M glycerol in the cell and this task has focused on efficient release of glycerol into the media. Methods tested included high temperature treatment, cell immobilization and mild sonication.

Deuterated membrane proteins

Membrane proteins perform a wide range of essential cellular functions and play a key role in e.g. transportation, energy management, signal transduction, photosynthesis. They are also implicated in a number of genetic diseases and have considerable therapeutic importance (70% of drug targets). This group has focused on the development of methods to optimise deuteration of membrane proteins. We have identified model membrane proteins and use bacterial expression systems in high cell density cultures for deuteration (fig 4). The deuterated membrane proteins will be used to reconstitute membrane systems with hydrogenated lipids for neutron studies and to test new classes of surfactants for their capacity to stabilize functional assemblies.

Deuterated lipids

One of the major limitations for the application of neutrons to the study of biological systems is the availability of deuterated lipids. Membrane biology is a particularly important area and a new range of powerful experiments could be carried out with the availability of selectively labelled lipids. The provision of unsaturated perdeuterated lipids with a range of head groups required the development of an optimised route for the production of oleic acid and conversion to the target lipids (fig

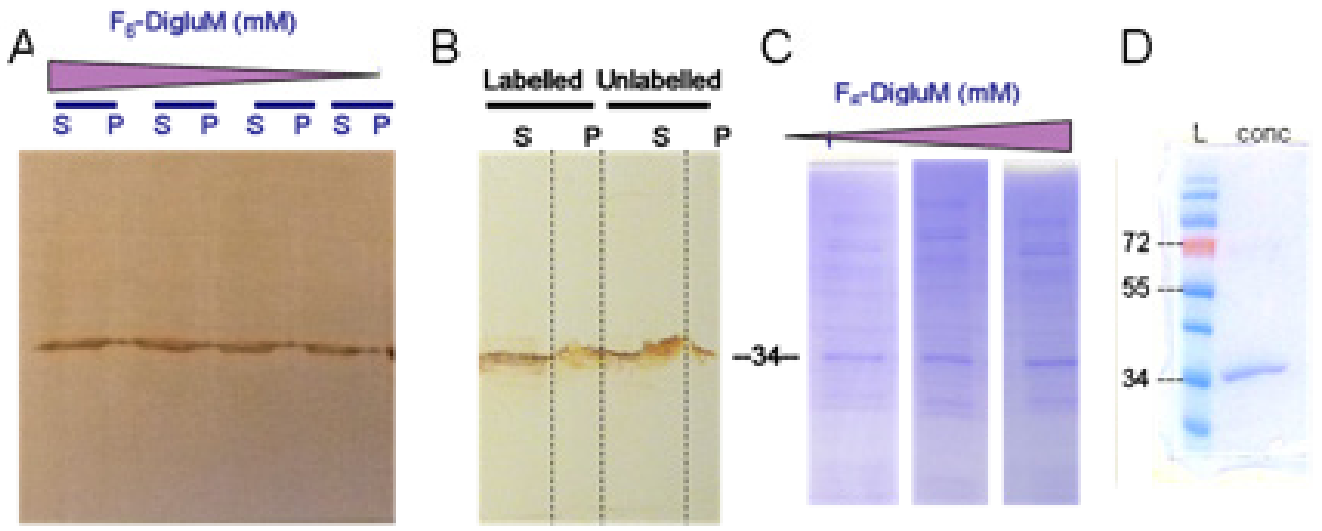


Fig 4. Screening experimental conditions for membrane protein synthesis: A. surfactant concentration in reaction mix. B. Deuterated versus hydrogenated amino-acids. C. Surfactant concentration in the feeding mix. D. Characterisation of the purified protein by SDS-PAGE.

5). We have developed a methodology for the production of full and part deuterated oleic acid. Coupling of the acids to phosphocholine head group is straightforward chemistry that is accessible to a wide range of academic and commercial groups. We plan to pass the material to a range of partners to both spread the load and develop a wider range of sources for the produced material. The phosphoglycerols (and phosphoserines) are synthetically accessible from the phosphocholines so these will be the main focus. Stockpiling of this material should enable milligram quantities of deuterated unsaturated phospholipids for use in neutron scattering experiments to be made available at relatively low cost.

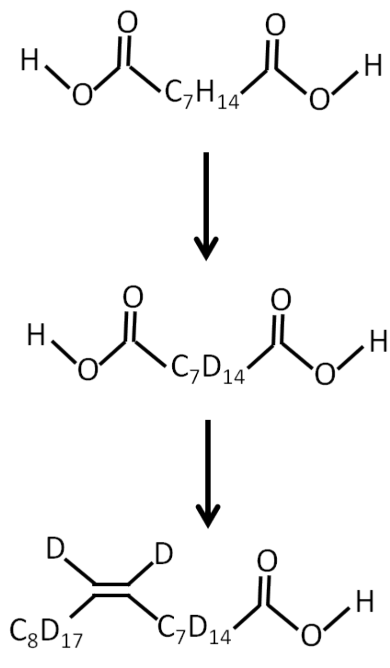


Fig 5. Main route to the production of deuterated oleic acid from azelaic acid to oleic acid

Conclusions and future work

The tasks carried out as part of this JRA have provided new capabilities in the area of biological neutron scattering and this is having a significant impact in widening capabilities throughout this part of the user community. For the future there are a number of key areas where further method development will be focused. For example we believe that major progress is possible for the culture of mammalian cells, cell-free synthesis, and in a number of key scientific areas such as the study of intrinsically disordered proteins, which play key roles in a vast range of physiological processes, and are also strongly implicated in important human diseases such as cancer and neurodegenerative diseases like Alzheimer's disease and prion-related diseases.

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Kennaway C. *et al.*, *Gene Dev.*, 26, 92-104D, 2012

The Polarised Neutrons JRA

Partners: Jülich Research Centre (FZJ) / Jülich Centre for Neutron Research (JCNS), Germany
Neutron Research Reactor Heinz Maier-Leibnitz (FRM II) , Germany
Technical University Delft (TUD), The Netherlands
Laboratoire Léon Brioullin (LLB), France
Technical University – Atominstitut Wien (TUW), Austria
St. Petersburg Nuclear Physics Institute (PNPI), Russia
Denmark Technical University (DTU), Denmark
Coordinator: Alexander Ioffe, Head at Outstation JCNS-FRM II

How did the idea for this JRA collaboration come up?
A collaboration on polarised neutron techniques was born over 10 years ago. It started within a European project called European Polarised Neutron Initiative - EPNI, which was organised and coordinated by Francis Tasset of ILL. This collaboration focused on two main topics: polarised neutrons and 3He neutron spin filters. Given the remarkable achievements of both topics, they resulted in two different JRAs: Eddy Lelievre-Berna became the coordinator of the Neutron Spin Filters JRA and I became the coordinator of the Polarised Neutron Techniques JRA.

What was it like coordinating collaboration between the different members of the JRA?
In 2004 it was the first time for this type of collaboration, so it took us some time to figure out how to work across facilities' interests and make the best out of the limited resources provided by NMI3. The funding period finished in 2008 and we realised that the results were very positive; we therefore decided to continue with the JRA throughout the NMI3-FP7 phase of funding. Given that we had worked together before and already knew the capabilities of each partner, the collaboration within the new JRA ran smoothly and everyone was able to contribute to the different tasks.

What have you and the others involved learned from this collaboration?
Brainstorming among partners fostered a sort of synergy effect. All partners learned that by working together in a friendly atmosphere we could learn a lot and receive important feedback to build new ideas and projects. This atmosphere definitely encouraged creativity in our research projects and had a positive impact on the development of new instruments that are now under construction or already in use in several facilities.
It is a big challenge to prepare a proposal for a 5-year period; in research we often obtain negative results that are also important. Not everything went as planned, some adjustments have been made on the way, and I appreciate very much the understanding of the European Commission with regards to this point.

What are the advantages of taking part in a project supported by NMI3?
While the financial support for such projects usually constitutes a small share of the resources required for completing a project, it actually helps to attract national resources. However, in my opinion, this is not the most important factor. NMI3's support stimulates collaborations, creating a momentum to generate new ideas for our research projects and it has consequently produced results. This support also allows the continuation of previous collaboration. Particularly in our work, we are still benefiting from the work done within the EPNI project that I have mentioned before. We have achieved remarkable results but I think that the main impacts of this JRA will be visible in the long-term, when the ideas we have developed will be used for construction of new instruments.

Will you continue participating in this type of collaboration in the future?
We decided not to continue this JRA during NMI3-II because we needed some time to look back on the work we have developed over the past 10 years, reflect about what has been done and think of new ideas for the future. The aim of the JRA was to provide connections, to initiate collaborations and these proved very successful. There is still space for new developments and I believe that the partners who are interested in collaborating will continue to do so. In the future, maybe in Horizon 2020, we might join efforts again to create a new polarised neutron JRA.

Polarised neutrons are particles with a preferential spin direction or magnetic moment and can be considered as the arrows of an elementary magnet. Similarly to classic magnet arrows placed in a magnetic field, their spin direction change when interacting with a magnetic dipolar field in the sample. These changes in the relative orientation can be measured very precisely using neutron polarimeters. Furthermore, the precession around the magnetic field's direction allows the attachment of a "Larmor clock", whose rotation speed depends only on the magnitude of the magnetic field of each neutron. Given that each neutron carries its own Larmor clock, the neutrons in the beam become distinguishable. This opens the possibility of developing unusual neutron scattering techniques, whose resolution does not require pre-defined initial and final states. Thus we can achieve an extremely high energy (or momentum) resolution that is not achievable in conventional neutron spectroscopy (or diffraction) because of intolerable intensity losses. This JRA aimed to develop an easily accessible wide-angle polarisation analysis technique for neutron diffraction/spectroscopy, and to extend the possibilities of Larmor labelling methods towards higher energy and momentum resolution. In this article we present only a few achievements of the Polarised Neutrons JRA. For a complete coverage please visit the NMI3 webpages.

Wide-angle neutron polarimetry

Large solid angle neutron polarimetry will allow the use of large solid angle detectors, which enable simultaneous data acquisition over a wide range of transferred momentum. This results in an enormous efficiency gain for neutron polarimetric experiments and opens new horizons for more detailed understanding of the mechanisms involved in multiferroic compounds, photo induced and molecular magnets, magnetic nanostructures, spin electronic and new superconductors, which are at the forefront of condensed matter research.

Within this task, we performed a detailed analysis of the different possibilities for the wide-angle analyser at the Super 6T2 diffractometer at LLB. We found that existing solutions employing the radial array of polarising supermirror (SM) analysers compete with similar devices based on ^{3}He spin filters only for long wavelengths. This considerably limits the application of SM analysers in single crystal diffraction and clearly favours the polarised ^{3}He technique for single crystal diffraction applications. This technique is based upon the strong spin dependent neutron absorption of the highly polarised ^{3}He gas, which makes it an effective neutron spin filter: it is transparent for neutrons with one spin direction and opaque for neutrons with the opposite spin direction. In the frame of the JRA, FZJ developed a very compact 70cm diameter magnetic system capable of producing a uniform field in three orthogonal directions over a very large solid angle (fig 1). The team also developed a pioneer method for manufacturing doughnut-like containers for ^{3}He gas from the dedicated GE180 glass.

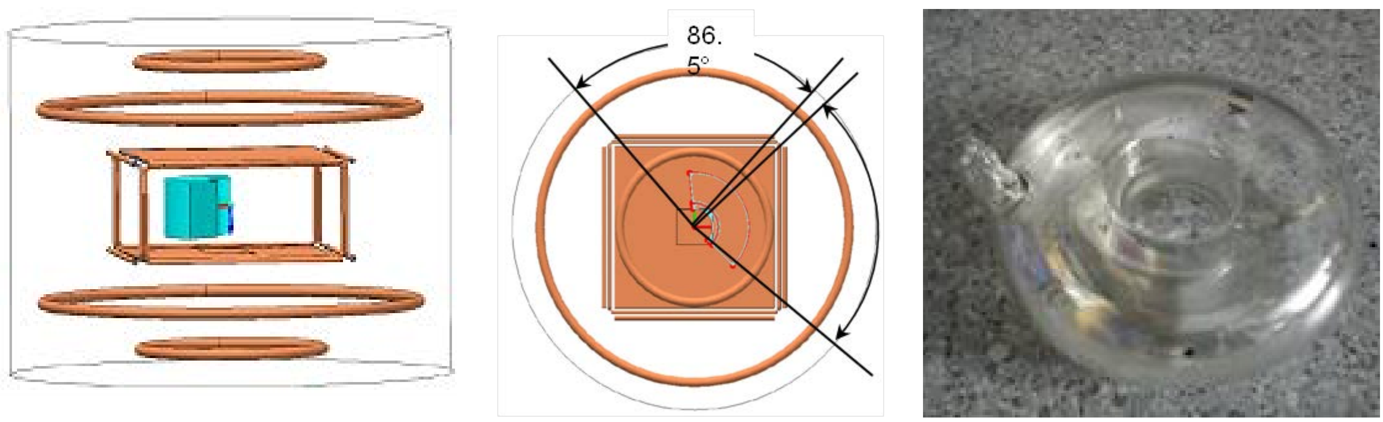


Fig 1. Very compact 70cm diameter magnetic system at FZJ (left) and the first in the world doughnut shaped cell with outer diameter about 20cm (right).

Larmor labelling methods for inelastic neutron spectroscopy, SANS, and reflectometry

Neutrons can be used to study dynamics on a molecular scale by measuring the neutrons' energy gain or loss during the sample analysis. Examples of these studies are the determination of lithium diffusion through a battery system or hydrogen transport through a fuel cell. Current instruments pre-select the incoming neutrons' energy, losing more than 95% of the available neutrons, and determine the scattered-neutron's energy by the time-of-flight (TOF) technique. A new TOFLAR technique, proposed in TU Delft, will use the whole neutron spectrum and determine the neutrons' energy by a modulation technique. By combining Larmor labelling and the TOF technique we will have a quasi-elastic neutron-scattering instrument with high neutron intensity and large accessible range of length and time scales on the molecular level. Within this task, the team of TU Delft has described the theoretical background, performed computer simulations, and a proof-of-principle experiment on a prototype instrument at the Reactor Institute Delft.

Neutron spin-echo spectroscopy is a method to analyse slow motions and relaxations on the length scale of atoms, molecules and molecular aggregates. In particular in soft-matter such as polymers, proteins and microemulsions, the combination of neutron diffraction (SANS) and spectroscopy with contrast generation by selective replacement of H-atoms by deuterium provides insight into the structure and mobility of these systems. The neutron spin-echo spectrometer has a unique resolution capable of detecting very small changes in the velocity of the scattered neutrons, about three orders of magnitude higher than that of any other neutron spectroscopic method. To further improve the resolution and the transmission of neutron-spin echo spectrometers, the team from FZJ has developed new correction elements that have a good transparency to neutrons and at the same time can withstand the large currents that are necessary to perform the correction. The challenge here was to combine good neutron transmission with high current density and a highly accurate distribution of electric current that is responsible for the corrective action. We have adopted an idea already employed at ILL for elements with smaller area and extended it to larger diameter and current density. These so-called "Pythagoras coils" consist of crossed current wedges (fig 2). Their combined action resembles that of a radial distribution. Despite the fact that their theoretical performance is somewhat non-ideal, they meet the theoretical expectation and they are the best performing correction elements that could be obtained up to now. Following this, we have produced a new design for the complete set of coils for the spin-echo spectrometer J-NSE in Garching, Germany, and the SNS-NSE at the JCNS outstation in Oak Ridge.

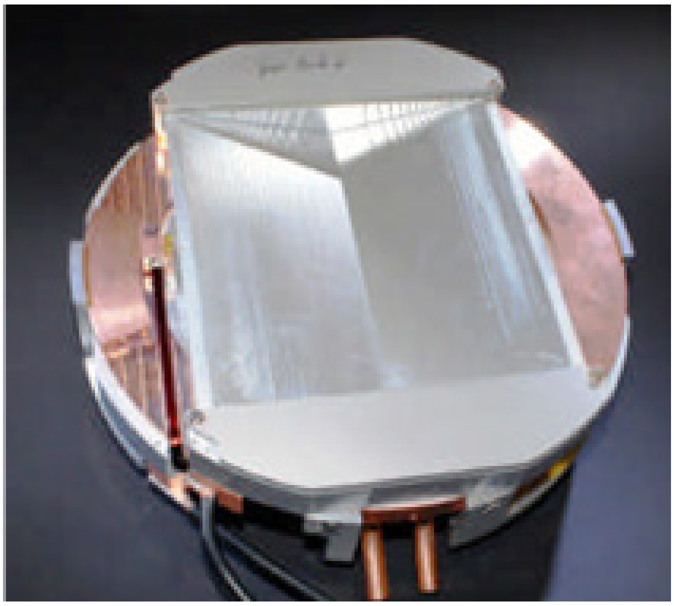
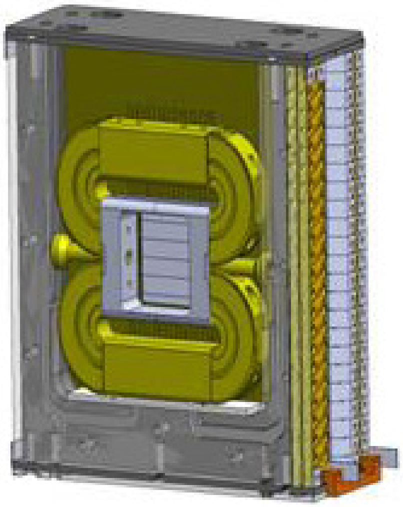


Fig 2. Crossed Pythagoras coils in FZJ

Monte Carlo simulations

Monte Carlo simulations are playing a very important role in the context of the design and optimisation of neutron scattering instrumentation. An accurate, carefully benchmarked computational model of a neutron instrument can underpin the design of new instruments and enhance the efficiency of existing ones. This makes the development of powerful Monte Carlo instrument simulation codes very important for the progress of neutron scattering research. A team at FZJ, in collaboration with the Joint Institute for Nuclear Research in Dubna, Russia, has extended the possibilities of the simulation software package VITESS allowing the simulation of spin dynamics in time-dependent magnetic fields. This paved the way for simulations of practically all existing spin-handling devices and Larmor-labelling neutron scattering instruments.



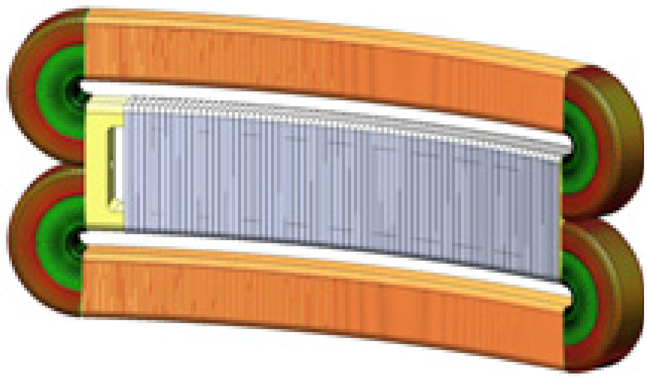


Fig 3: Flat Neutron Resonance Spin Echo (left) and curved Radio-Frequency (right) coils for the primary spectrometer at LLB

Large Solid Angle Resonance Spin-Echo

The aim of this task was to design, develop and construct Large Solid Angle (LSA) coils for a neutron resonance spin echo spectrometer. In a first phase, we used two flat LSA coils for the primary spectrometer, each of them including two radiofrequency coils inserted in static coils (fig 3 left). For the secondary spectrometer, in order to achieve a measurement over a very wide angle, a curved coil has been developed with the aim of simultaneously covering 15° of the scattering angle (fig 3 right). In another approach developed at TUM, the curved coils are not winded to a body, but cut from a single aluminium piece by means of electrical discharge machining. The coil design and the construction were performed at LLB and TUM and the test has been carried out on the spin echo spectrometer G1bis at LLB.

Measuring triplet correlation functions

Nowadays neutron experiments can determine the mutual position of two scattering objects in the sample: the distance between these objects is the length scale at which we probe the sample (the so-called pair correlation function). However, through the Neutron Resonance Spin Echo (NRSE) technique, one can split the initial neutron wave into four waves corresponding to three different distances so that the neutron waves probe the sample simultaneously on three length scales. The detected intensity will now depend on distances between three scattering objects in the sample (so-called triplet correlation function). The prototype setups for the Four-Wave NRSE experiments and Spin-Echo Small Angle Neutron Scattering (SESANS) have been built at the reactor of PNPI in Gatchina, Russia.

Ultra-Small-Angle Polarised Neutron Scattering

The characterisation of the magnetic structure of matter and the study of its evolution under varying external conditions is a particular strength of neutron research. A new option for investigating the magnetic microstructure is the Ultra-Small-Angle Polarised Neutron Scattering technique (USANSPOL), which relies on the high resolution of scattering angles provided by perfect crystal neutron reflection. ILL has set up an instrument configuration for this (fig 4). The instrument was equipped with magnetic prisms for neutron polarisation and a dedicated sample environment. The sample environment provides 3D control of an external magnetic field configuration ranging from a zero-field environment via continuous intermediate setups to the magnetic saturation of the samples. In addition, this sample environment enables us to apply external mechanical forces for the study of magnetostriction in novel technologically relevant materials used in modern sensors and actuators. Our test experiments demonstrated the potential of this new technique. It offers a picture of the structure that may be related to material functionality and may eventually lead to technological improvement.

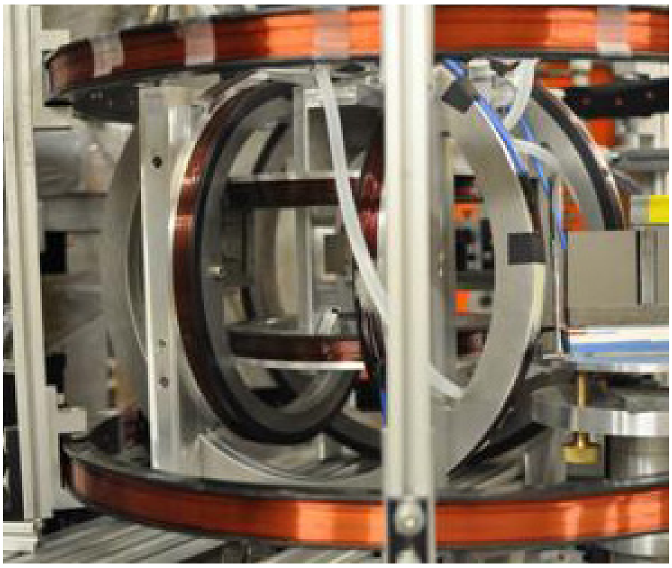


Fig 4. USANSPOL sample/analyser crystal area in S18 at ILL

Ultra-flexible neutron magnetic resonator

The spectral and temporal tailoring of neutron beams is an important issue for advanced neutron sources like the European Spallation Source. Spatial magnetic neutron spin resonance as the basis for the famous Drabkin-resonator demonstrated its potential for defining the spectrum of a polarised neutron beam as early as the 1960s. With the novel idea of controlling each element of the neutron resonator separately, a concept was invented that allows for polarised neutron beam tailoring of unprecedented flexibility regarding key parameters like incident and final neutron energy, spectral width of the incoming beam, or its energy resolution. We have built two prototype resonators based on the same principle and tested them experimentally at a polarised neutron beam line at the Atominstitut TRIGA reactor of the Vienna University of Technology (fig 5). The experiments demonstrated a flexible spectral definition of the neutron beam with variable resolution in continuously operated mode, applicable in diffraction and fundamental physics experiments. For the first time, the team also performed a travelling wave mode of operation where short neutron pulses in the microsecond range are produced by synchronised magnetic field pulses. This offers new possibilities for neutron spectroscopy as it decouples the energy resolution from the TOF resolution of the neutron beam. In addition, a Ramsey-type resonator setup was conceived and tested which offers promising potential for advanced neutron spectroscopy techniques.

Conclusions

In the past, neutron polarisation experiments were considered delicate, difficult to understand, and often too costly in flux. The work carried out within this JRA has clearly extended the power of polarised neutron scattering for delicate experiments investigating the nature of magnetism and magnetic phenomena in solids. Much can still be done to enhance polarised neutron techniques. We will now take time to reflect on the work developed over the past 10 years, but we believe that the possibility of forming a new Polarised Neutrons JRA in the future cannot be discarded.

Relevant publications

M.Bleuel *et al.*, *Physica B*, V406, 2011
E. Knudsen *et al.*, *Physica B*, 2011
G. Badurek *et al.*, *Physica B*, V406, 2011
Yu. O. Chetverikov *et al.*, *X-ray, Synchrotron and Neutron Techniques*, Vol. 5, No. 4, 2011
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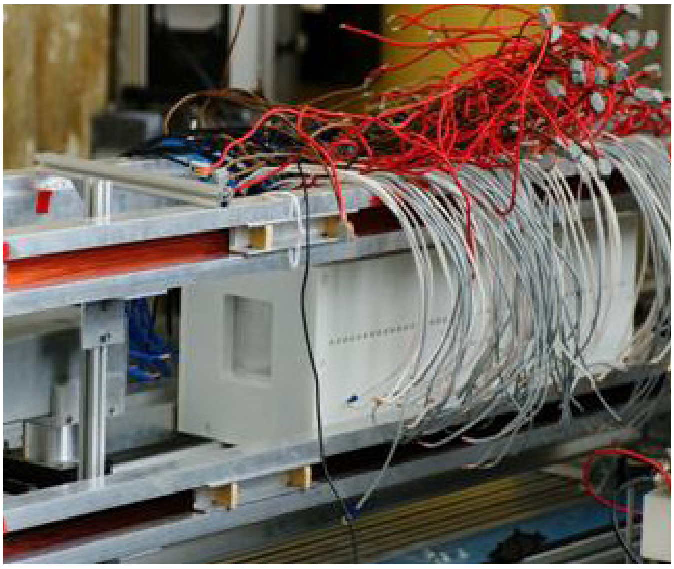


Fig 5. Prototype 2 spatial magnetic spin neutron resonator at TUW

Joint Research Activities

The Neutron Optics JRA

Partners:

Laboratoire Léon Brillouin (LLB), Institut Laue Langevin (ILL), France

Budapest Neutron Center (BNC), Hungary

Matter Physics National Institute (CNR – INFM), Italy

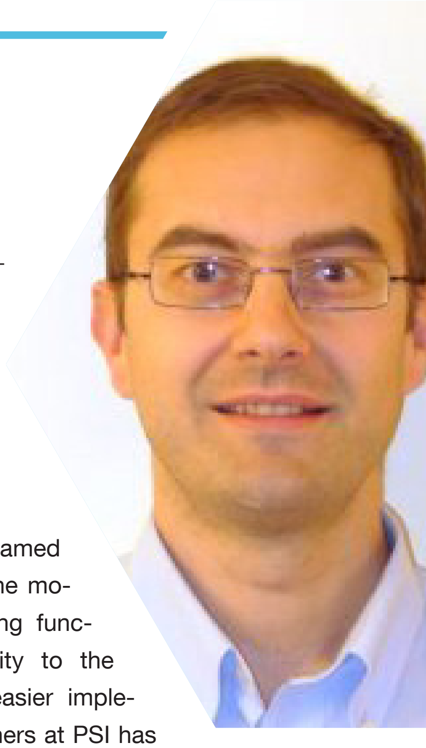
École Polytechnique Fédérale de Lausanne (EPFL) and Paul Scherrer Institute (PSI), Switzerland

Jülich Center for Neutron Scattering (JCNS), Helmholtz Centre Berlin (HZB), and Technical University of Munich (TUM), Germany

Nuclear Physics Institute (NPI), Czech Republic

University of Copenhagen (UCPH) and Denmark Technical University (DTU), Denmark

Coordinator: Frédéric Ott, instrument responsible at LLB



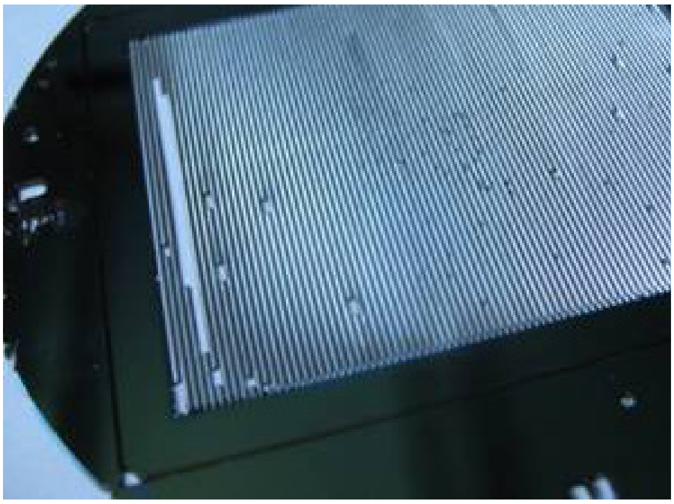
The field of Neutron optics is revolutionising neutron scattering in the same way as the telescope empowered the astronomer's naked eye. Thanks to the technological advances made over the last decade, a number of optical concepts that were impossible to exploit until recently can now be applied to neutron optics. The aim of this JRA was to develop new optical components for neutron scattering spectrometers. Neutron scattering used to be the realm of large samples (1cm^3). It is now possible to analyse sub-mm samples, and imaging at the µm scale will soon be within reach.

High flux reflectometry and energy analysis

One of the first tasks of this JRA was to investigate the possibility of increasing the efficiency of neutron reflectivity experiments. Several routes were proposed to enable the use of a very large part of the total flux available in the neutron guides.

The first route aimed at using reflective optics. The initial project was based on the REFOCUS concept, which has been upgraded. The new scheme named SELENE involves separating the monochromatisation and focussing functions, providing more flexibility to the design together with much easier implementation. A group of researchers at PSI has produced a prototype SELENE bench at half scale. The gains in flux obtained are of the order of 10 with respect to a conventional set-up.

In the second route, our JRA proposed that the energy analysis of a white neutron beam could be performed using the refraction in a prism. A large MgF_2 crystal was bought by ILL in order to build an energy dispersive spectrometer. This provided data of a quality similar to time-of-flight data and can be easily implemented on any time-of-flight reflectometer. In high-resolution experiments it is possible to achieve gains in the range of 30-90. This can be useful for kinetic experiments or for measurements on small samples. To improve this set-up,



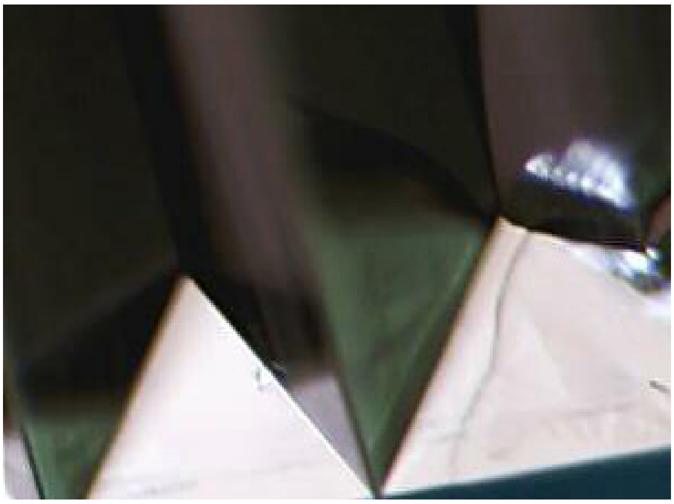


Fig 1. Silicon wafer in which Si prism has been etched (left) and zoom on one of the prisms (right)

HZB developed a technique for manufacturing arrays of silicon prisms using a chemical etching process. This allows perfectly aligned and smooth silicon prisms to be produced (fig 1). The use of several dozen prisms makes it possible to multiply the refraction effects by the number of prisms, thus proportionally increasing the deflection angles. A wafer of these prisms was stacked and characterised on the EROS reflectometer at LLB; it could be confirmed that they do behave as energy analysers.

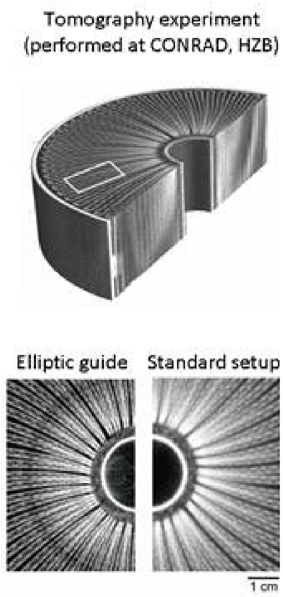


Fig 2. Tomography experiment performed with and without image magnification.

Advanced focussing techniques

Phil Bentley has developed genetic algorithms for the optimisation of neutron optics. The use of genetic algorithms has shown that it would be possible improve the efficiency of focussing guides by 30%.

Some new McStas components were successfully used to model adaptive optics. A 1D parabolic focussing system has been extensively modelled using and a number of full-scale adjustable focussing devices were built and tested. The results agree with the numerical simulations. Two prototypes were built: one with an adjustable focal point and another with five motors to tune the mirror shape. Appropriate control software was written to be able to change the shape of the mirror without breaking it. A more advanced 2D focussing device was built for the instrument TOF-TOF at FRM II, enabling the curvature of the super-mirrors to be changed as a function of wavelength, in order to keep the focal point at the sample position. The team thus managed to double the flux at the sample position.

High resolution imaging using reflective optics

A group of scientists from this JRA has demonstrated using Monte-Carlo calculations that elliptic neutron guides lead only to minor distortions of the phase space and can therefore be used efficiently for neutron radiography and tomography. The group performed Monte-Carlo simulations for various imaging geometries using a straight guide, a convergent guide and an elliptic guide. It used a small section of an elliptic guide to demonstrate the principle of image magnification to achieve gains in spatial resolution. A significant improvement in image resolution was obtained, as shown in figure 2.

The neutron optics group at HZB led by Thomas Krist has designed and built a new type of high-resolution neutron-imaging detector. The small pixel size of the detector requires a high flux density for imaging experiments. The group has designed and optimised Kumakhov-type lenses for improved neutron beam focussing; these have provided a flux gain of 20x, allowing realistic exposure times of several minutes.

The new imaging facility CONRAD-2 was designed at HZB. This imaging facility using reflective optics provides a beam quality that can be used for imaging purposes. In future investigations the last guide section of the facility could be replaced by a focussing guide to re-assess the parameters of the facility.

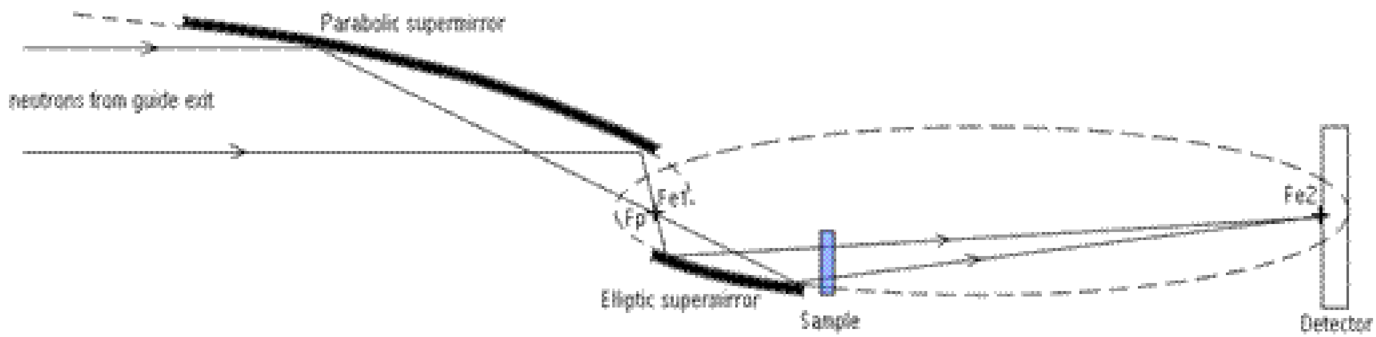


Fig 3. Design of the focussing device with a combination of parabolic and elliptic SM

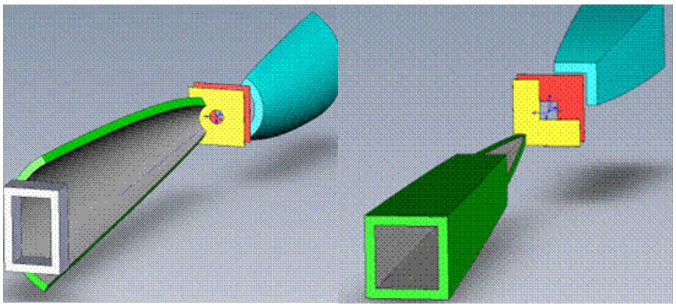


Fig 4. A two dimensional setup (left) and a 1D+1D setup (right).

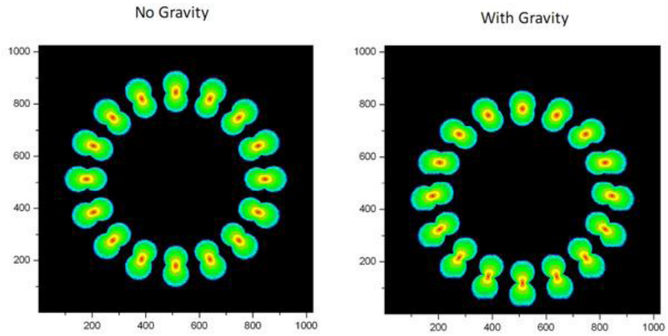


Fig 5. Calculation of the resolution function of a SANS diffractometer with refractive lenses (gravity taken and not into account).

Focussing SANS using reflective optics

The aim here was to design a focussing system on SANS spectrometers using an achromatic combination of curved supermirrors with no absorption (fig 3). SANS instruments could benefit from this technique in terms of flux at the sample. A test bench was produced at LLB and tested at PSI in September 2011 on the optical test beamline BOA.

The current device only provides improved performance in one direction. The overall set-up would perform better if focussing was possible in two directions, as shown in figure 4. This type of set-up is not technically feasible today. For this reason, a team of researchers tested the optical components of such a set-up on the optical beamline at BNC. Whilst the device provides roughly the expected performances, the optical imperfections observed are too large for SANS experiments. Thus for the new focussing SANS instrument at BNC, a Kirkpatrick -Baez arrangement combining two 1m-long elliptical mirrors will be used.

Focussing SANS using refractive optics

Using refractive lenses to implement focussing SANS could make it possible to measure scattering patterns down to much smaller Q values. JCNS has been working on this concept. The first issue was the production of aspherical lenses, to avoid aberrations for large diameter lenses. JCNS therefore ordered Zeiss MgF_2 lenses. The second issue was that phonon scattering significantly reduces the transmission of these lenses at room temperature. A group of scientists therefore built a dedicated cryostat to accommodate three lens stacks. Thirdly, there was a need for the appropriate data processing tools. The group performed Monte-Carlo simulations to quantify the aberrations introduced by the lens system (fig 5) and concluded that optical artefacts from the lenses are negligible when compared to gravity effects. In parallel, the group upgraded the data processing programs for the three SANS instruments, to calculate the resolution effects for SANS measurements. The package qtiKWS developed by V. Pipich treats all SANS data; the internal SANS data of JCNS instruments KWS-1, KWS-2, KWS-3 is preferred.

Modelling of interacting optical elements

There was a wish among users to avoid writing new components to describe new geometries / devices, given that there are already many useful components to build from. The problem is that McStas intrinsically uses a linear flow. Here we devised a solution to handle the assembly of basic optical elements to build a new McStas component. The technique was demonstrated on a “meta-component” including a guide with an embedded, wedged, polarising mirror system of the same type as the one at HZB.

Optical simulation workshops

Peter Willendrup, Linda Udby, Klaus Lieutenant, and Emmanuel Farhi organised a McStas/VITESS school in May 2010 on Ven in Sweden. Later in 2011, the group held another workshop on a more specialised use of McStas. The partners of the projects contributed several components to the McSTAS library.

Recent publications

Desert S., Panzner T., Permingeat P., *J. Appl. Crystallogr.*, 46(1), 35-42, 2013

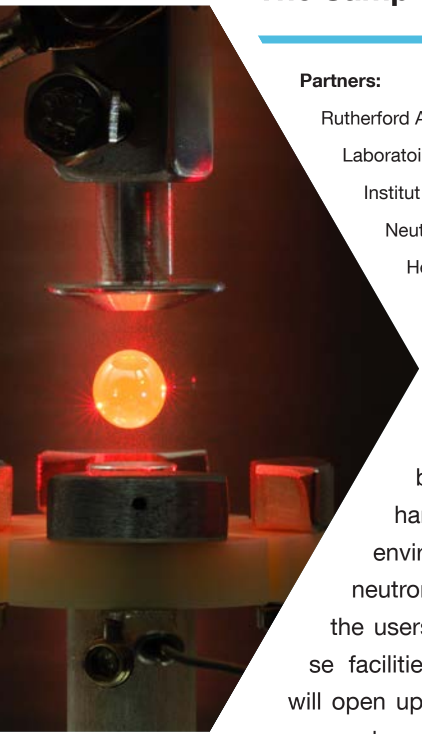
Mikula P. *et al.*, *J. Appl. Crystallogr.*, 46(1), 128-134, 2013

Stahn, J.; Filges, U.; Panzner, T., *Eur. Phys. J. Appl. Phys.*, 58, 11001, 2012

P.K. Willendrup *et al.*, *Nucl. Instr. Meth. A* 634, S150-S155, 2011

R. Cubitt & J. Stahn, *Eur. Phys. J. Plus* 126, 111, 2011

The Sample Environment JRA



Partners:

Rutherford Appleton Laboratory (ISIS), UK

Laboratoire Léon Brillouin (LLB), France

Institut Laue-Langevin (ILL), France

Neutron Research Reactor Heinz Maier-Leibnitz (FRM II), Germany

Helmholtz Centre Berlin (HZB), Germany

Coordinator: Zoë Bowden, Division Head at ISIS

The Sample Environment JRA is a far-reaching collaboration whose aim is to enhance the capabilities of sample environment available at European neutron facilities, in order to expand the users' research possibilities in these facilities. New sample environments will open up new territories for hydrostatic pressure, temperature and advanced gas adsorption facilities, pushing at the boundaries of *in-situ* experimentation. Significant progress has been made in overcoming the technical challenges associated with these advances in sample environment. This has been greatly aided by the continual sharing of knowledge and experience between the technical groups at member facilities. This JRA provided a breath-taking array of new sample environment equipment and experience in much desired but technically very challenging areas, opening up new realms of scientific exploration.

High pressure gas cells

High-pressure research is one of the fastest-growing areas of natural science, and one that attracts such diverse communities as those of physics, bio-physics, chemistry, materials science and earth sciences. In condensed matter physics there are a number of highly topical areas such as quantum criticality, pressure-induced superconductivity or non-Fermi liquid behaviour, where pressure is a fundamental parameter. An increase in the range of available pressures up to 10kbar for gas-loaded cells makes a significant impact on the range of science possible at neutron facilities. However, high pressure gas sample cells require thick cell walls which may lead to an unacceptable neutron background and thus the choice of materials and geometries is critical to improving the quality of the data. Reliable, safe and user-friendly high pressure gas handling systems are also an essential part of the development.

Fig 1. Pressure cells

The aim of this task was to provide a range of containers (cells) for high pressure gas samples and suitable pressure-generating equipment. An extensive investigation into potential materials was carried out, supported by material testing carried out by students at Imperial College London. To complement the test data the collaboration used experimental results from the Engin-X diffractometer at ISIS and extensive finite element analysis (FEA) to aid design. All the cells specified were made and tested successfully (fig 1). Most were made from beryllium copper, but for high temperature 4 kbar hydrogen Inconel was used because the data showed that beryllium copper is not suitable at elevated temperatures. For 8 kbar hydrogen a composite cell with a hydrogen-resistant beryllium copper liner and a neutron-transparent outer of titanium zirconium was used in order to increase the neutron transmission through the cell. To enable the full exploitation of this suite of high pressure cells, a support network of safety features, testing facilities and gas handling systems was also produced. This equipment included gas 'intensifiers', which compress the gas to pressures over 10 kbar - 10,000 times atmospheric pressure. The ISIS test area was updated and strengthened, and has already been used by LLB. The LLB produced a cryogenic system in order to fully test their cells at low temperature. LLB and ISIS procured

10 kbar inert gas intensifiers and ISIS extended the range of their hydraulic intensifier to over 13 kbar. Both the HZB and ISIS constructed 10 kbar hydrogen intensifiers (fig 2). These new pressure cells and equipment have doubled the pressures available to LLB and ISIS users. Several of the cells have already been successfully used for experiments at ISIS and HZB.

High temperature furnaces

Studies of the liquid state are not only significant from a fundamental point of view but also represent important technological interests. The molten state is an essential stage in various industrial processes. However, the study of structure and dynamics in liquid metals or dielectric materials is often prevented by the chemical reaction of the high temperature melt with its sample holder. As part of this JRA, two furnaces were developed for different sample types: an aerodynamic version at the ILL and an electrostatic version at FRM II. An aerodynamic furnace uses high speed gas jets to suspend the sample; an electrostatic furnace levitates charged samples using electric fields. Existing aerodynamic furnaces were not suitable for experiments on neutron beamlines because of sample instability and sample access: only two-thirds of the molten sample volume was generally visible to the neutron beam. The neutrons scattered by the nozzle also created unwanted background scatter, leading to data analysis problems. These were significant problems to overcome but after many trials of different gas nozzle types, geometries and flow rates, a solution was found. The novel four-nozzle technique developed allows the stable levitation of a sample up to 6 mm in size, unobscured by the nozzle. It is also now possible to change the atmosphere in which the sample is heated, for example by the introduction of a small proportion of oxygen or carbon dioxide. Figure 3 shows a levitated sample during heating. Experiments may now be carried out at temperatures up to 3000 K, a temperature never before obtained on a neutron beamline.

Fig 2. ISIS 10 kbar hydrogen gas intensifiers

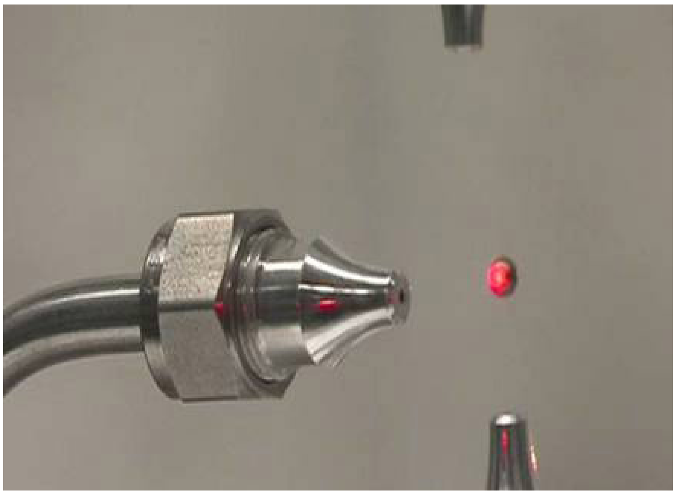


Fig 3. Laser sample heating in levitation furnace

The main task facing the FRM II team working on the electrostatic furnace was to adapt an existing system to fit the spatial constraints of a neutron scattering instrument. The system also needed an upgrade to levitate the larger samples required for the neutron beam, as well as improvements to portability, reliability and user handling. Working in partnership with the German Aerospace Centre (DLR) an improved and compact furnace has been made. It has been tested and used for neutron scattering experiments on beamlines at both the FRM II and ILL. The system has fulfilled all its specifications and the addition of a laser pre-heating stage now removes unwanted organic material from the surface of the sample as well as dissolved gases and other contamination of the bulk material. This results in a more reliable and faster melting process and aids the processing of new sample systems.

Gas Adsorption Control Systems

Gas adsorption is the process by which components of a gas adhere to the surface of a sample. Volumetric analysis determines the extent of adsorption by measuring the change in sample volume; gravimetric analysis by measuring the change in sample weight. The technique of gas adsorption is very important for the measurement of hydrogen storage materials and the characterisation of chemical and catalyst reactions in porous materials.

The greatest challenge to the HZB team was overcoming the complexity of automating the supply of an accurate measure of gas to the sample for the adsorption process. The difficulties of providing a range of multipurpose apparatus, suitable for neutron beamline use, which was safe, user-friendly and flexible were also significant. New construction materials had to be investigated and were rigorously tested under extreme conditions before approval. Important safety measures had to be taken to provide protection against possible material failures. To avoid compromising accuracy or performance, specialised equipment was developed for specific sample conditions. The range in volumetric systems was initially increased with the development of systems for the in-situ measurement of gas adsorption at a specific temperature, at low pressure and in the temperature range 1.5 to 600 K. New equipment includes a cryo-furnace insert and a mini mechanical cooler version for use on neutron beamlines with restricted access. In addition, we have developed accessories to facilitate the supply of gas to the sample including a glove-box insert and a self-locking sealed sample can. We then built a gas handling system with automated control, operating at up to 200ºC and 300 bar. This comprehensive system incorporates an oven to heat the gas supply tubes to the sample, ensuring that the vapour condenses in the correct place for analysis. A residual gas analyser has also been adapted for the system to provide chemical composition information for experiments related to reactions and catalytical processes. This gas handling system has been in successful operation for experiments since July 2012.

For gravimetric analysis we have adapted an existing magnetic suspension balance for neutron scattering experiments. A magnetic suspension balance weighs samples without contact, separating the weighing instrument from the sample which may be in a corrosive atmosphere or under extreme temperature and/or pressure conditions. Firstly, to guarantee a reproducible sample position with respect to the neutron beam, a mechanical depositing rack has been added. Secondly, a high pressure hydrogen vessel for the balance has been designed and made, incorporating a hydrogen-resistant liner and a neutron-transparent outer casing. Thirdly, a control system allowing the application of either variable gas mixtures or humidities has been developed. This system can remotely regulate the gas flows, the temperature (to 500ºC) and the

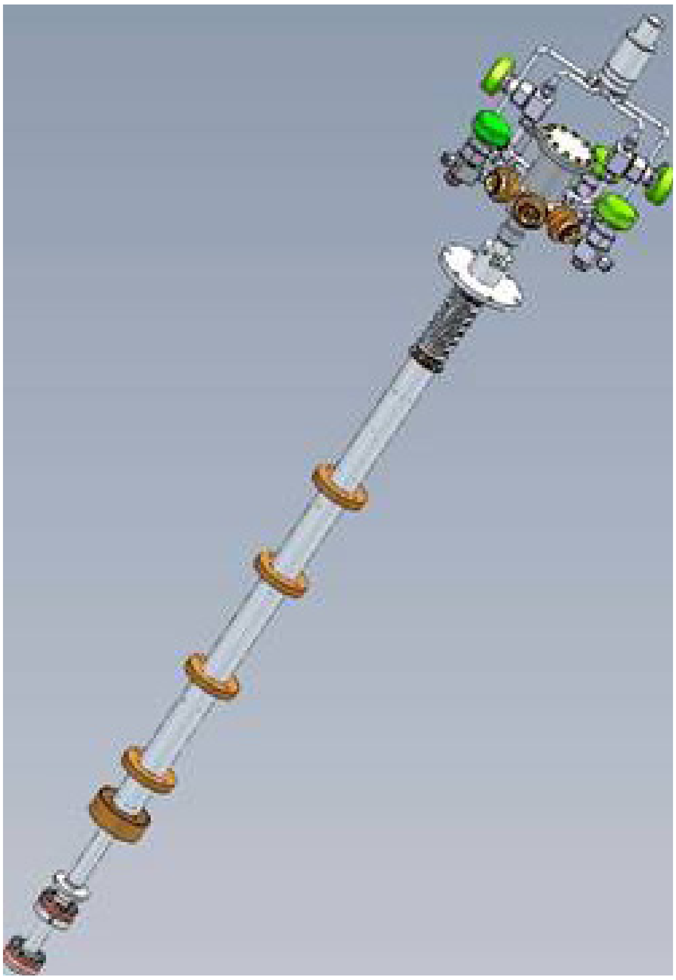


Fig 4. Gas handling - unified sticks

pressure (0.5-35 bar) of the sample container on the balance. To this was added a high pressure (up to 300 bar) gas handling system, built together with an industrial partner, which allows very precise sample pressure control. Finally, the working range for gravimetric analysis on the neutron beamline has been extended still further down to cryogenic temperatures, -250ºC and below. A customised helium flow cryostat had to be designed as no existing system was suitable. The sample holder is cooled by contact with the cryostat heat exchanger and magnetically coupled to the suspension balance by a thin fibre to minimise heat transfer, and then lifted for sample weighing. A series of thermal radiation shields helps to maintain a constant temperature around the sample whilst allowing almost 360º neutron beam access to the sample. The advanced performance and automated control of these adsorption systems has successfully increased the rate of experiments at the HZB.

In addition, to complement the equipment described above, the ILL, in cooperation with HZB and ANSTO, Australia, has developed an improved version of a gas adsorption stick. This stick combines volumetric, continuous flow and gas mixing applications together with a standard sample cell design (fig 4). This stick is easy to use and maintain, and provides users at different neutron facilities with a standardised piece of equipment. It has already been successfully used in several experiments.

Impacts on science

The greatest impact this sample environment JRA will have is on science – moving boundaries and extending experimental ranges. For example, the advances in high pressure equipment will enable further exploration in the areas of condensed matter physics, planetary and geo-science - studies of high pressure gases, which mimic conditions on other planets or inside our own - and high pressure hydrogen research, which may yet provide the answer to global energy problems.

The development of two types of levitation furnace will allow studies of high temperature melts across a broad range of both conducting and non-conducting materials not possible before. Studies of the molten state are not only of interest for fundamental research, but are also very important for technology. It is an essential stage in various industrial processes such as glass-making, semiconductor technology and iron and steel production.

The suite of new gas adsorption equipment will contribute significantly to many areas of science including the development, characterisation and improvement of proton conducting materials, gas sensors, nanostructured porous materials and catalytic converters. This will aid research into improved drug delivery, hydrogen storage solutions and catalysts used to speed up industrial and chemical processes.

Impacts on industry

The availability of high pressure, hydrogen-certified parts is now much improved thanks to the broader market opened up by the JRA. Through the continued requests of the JRA partners, European suppliers of high pressure equipment recognised the need for the development of products like valves, fittings and transducers guaranteed for work at high hydrogen pressures. In addition, a number of companies are now more aware of the common needs of the sample environment community, leading to mutually beneficial developments and a consensus on standards.

The beginning of a fruitful collaboration

The JRA project has led to radical changes to the relationship between the sample environment teams. Now, a well-defined international sample environment community exists. The European partners have led the way with the formation of a global society, the SE@NSF. There is now a forum for sample environment discussion shared by almost 40 collaborators worldwide, including those at facilities in Japan, USA and Australia. Information-gathering visits with specific aims have already taken place between facilities. Leaders of the neutron institutes recognise that collaboration by technical teams, such as sample environment, should be supported as it makes for a highly effective use of resources and promotes elevated standards across the neutron facilities.

Recent publications

E. Mac *et al.*, *Int J Hydrogen Energy* 37, 2012
K. Kamazawa *et al.*, *Adv Energy Mat,* 2012
M. T. F. Telling *et al.*, *Phys. Rev. B* 85, 2012
M. Sharif *et al.*, *J. Nanotechnol.* 3, 428, 2012
P. Kalisvaart *et al.*, *J. Phys. Chem.* 116, 5868, 2012
M. Erko *et al.*, *Phys. Chem. Chem. Phys.* 14, 3852, 2012
T. Kordel *et al.*, *Phys. Rev. B* 83, 2011
F. Yang *et al.*, *J. Phys.: Condens. Matter* 23, 2011

Using muons to measure spin polarisation in organic spin-based devices

By A. Drew, University of London

Information and Communication Technology

Spintronic devices, electronic devices that utilise the spin degree of freedom of electrons, hold unique prospects for future technology. Research by Dr A. Drew and colleagues shows that it may be possible to use spintronics to develop faster, smaller computer chips, combining processing power and memory.

Measuring spin

The most common method for using the spin in devices is based on the alignment of the electron spin relative to either a reference magnetic field or the magnetisation orientation of a magnetic layer. Device operation normally proceeds with measuring a quantity, such as the electrical current, that depends on how the degree of spin alignment is transferred across the device. The electrical resistance of the device then depends on the reference magnetic field, or magnetisation orientation, a phenomenon known as magneto-resistance. The so-called "spin valve", shown in figure 1, is a prominent example of such a spin-enabled device that has already revolutionised hard drive read heads and magnetic memory. The reduction in spin polarisation in the yellow spacer layer is governed by the "spin penetration length", which is related to intrinsic spin relaxation mechanisms in the spacer layer.

Understanding the transfer of spin polarisation in real device structures remains one of the most difficult challenges in spintronics because it depends not only on the properties of the individual materials that comprise the device, but also on the structural and electronic properties of the interface between the different materials.

Measurements on LE-muSR

Thanks to NMI3 funding, we used the Low Energy Muon Spin Rotation (LEmuSR) spectrometer of the Paul Scherrer Institute in Switzerland to perform a depth-resolved measurement of the spin polarisation of current-injected charge carriers in an organic spin valve. Crucially, the measurements were carried out below buried interfaces of a fully functional technologically realistic device. This enabled the correlation of the device magneto-resistance and the measurements of spin penetration on the nanoscale. The results suggest that the spin diffusion length is a key parameter of spin transport in organic materials.

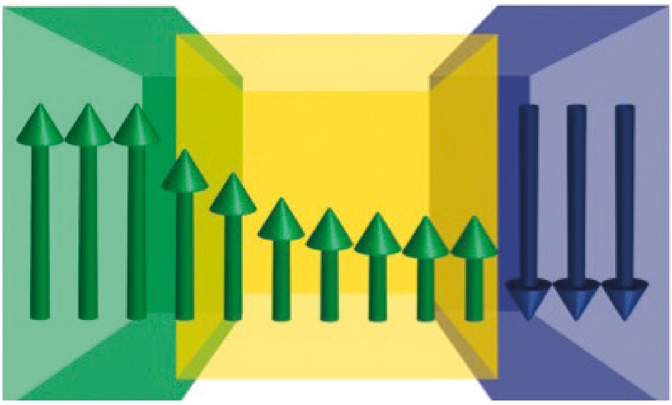


Fig 1: An archetypical spintronic device: the spin valve.

LiF reverses spin polarisation

In an extension to this work on spin penetration in the spacer layers, our group investigated how to engineer the magnetic, semiconducting interface to reverse the spin polarisation of the charge carriers in the device. We did this by including a very thin (1nm) layer of Lithium Fluoride between the ferro-magnet and organic semiconductor. The team observed that the lithium flouride layer at the interface reverses the spin polarisation of the charge carriers and therefore changes the sign of the magneto-resistance. This opens up the possibility of an electrically controllable spin valve.

These results highlight the unique potential of the LEmuSR technique to reveal the role of the various mechanisms that limit the spin coherence, especially in systems involving organic materials.

Original Publications

A. J. Drew *et al.*, *Nature Materials* 8, 109-114, 2009

L. Schulz *et al.*, *Nature Materials* 10, 39–44, 2011

Alan Drew from the Condensed Matter Physics Group at the School of Physics of Queen Mary, University of London and Francis Pratt from ISIS received NMI3 support to perform experiments at PSI.

Using muons to determine the role of Hydrogen impurity in oxides

By R. C. Vilão, University of Coimbra

Information and Communication Technology

Transistors are key components of computer chips. Our ability to develop transistors of ever-decreasing size underpins the future of computing. However, transistor miniaturisation is currently facing fundamental obstacles as these components reach atomic dimensions. One of the problems is the reduced thickness of the insulator layer of silicon dioxide SiO_2 used in the gate of transistors because it can be conductive, which can prevent the device from operating. The capacity of insulators to respond to an applied electric field can be quantified in a parameter called the dielectric constant. A possible solution to the problem of insulator thickness is the replacement of SiO_2 by more 'robust' insulators with a higher dielectric constant. In this context, the investigation of the role of hydrogen as an impurity has become increasingly important, especially since the discovery that this ubiquitous impurity may play a role in electron conductivity in zinc oxide.

We have addressed the characterisation of the isolated hydrogen configurations in paratellurite (α-TeO_2), an interesting and relevant semiconducting oxide for optical devices. The presence of hydrogen in the fabrication process of this material leads to hydrogen incorporation in the lattice, and therefore we were interested in investigating the effects of this incorporation in the electrical properties of this material.

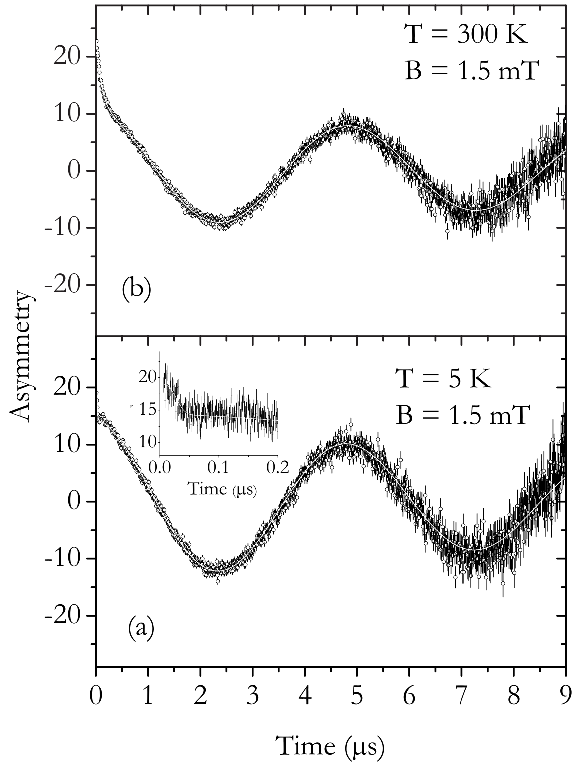


Fig. Muon spin asymmetry as function of time

Using muonium to characterise hydrogen states

From the experimental point of view, the use of muonium, an atom composed of a positive muon as the nucleus, as a light pseudo-isotope of hydrogen has become standard in order to obtain information about the electronic states of hydrogen in materials. We have thus performed muon-spin research (μSR) experiments at the ISIS Facility, United Kingdom, and at the Muon Spin Laboratory at the Paul Scherrer Institut, Switzerland. Our measurements enabled us to extract information about the muonium atom location and dynamics.

H as an amphoteric impurity in TeO_2

The results obtained in association with *ab initio* calculations clearly identify the basic donor and acceptor configurations of isolated hydrogen in TeO_2 (e.g. see figure). Moreover, the corresponding levels are suggested to be inverted in the band gap, so that the binding energy of the second electron in the H- configuration is larger than the binding energy of the electron in the H0 configuration. As a consequence of this inversion of levels, if the material is electron-deficient, hydrogen will tend to donate its electron to the conduction band, acting as a donor. If the material is electron rich, hydrogen will tend to capture an extra electron from the conduction band, behaving as an acceptor. In short, hydrogen will tend to always counteract the prevailing conductivity, and to act as an amphoteric impurity.

Original publication:

R. C. Vilão *et al.*, *Phys. Rev.* 84, 045201, 2011

Rui Vilão, Ricardo Vieira and João Gil from the University of Coimbra received NMI3 support to perform experiments at PSI.

Remediation tools for conservation of artworks

By Piero Baglioni, University of Florence

Cultural Heritage

In the past, synthetic polymers have been improperly applied as protective coatings to painted surfaces. Instead of preserving the paintings, these substances promoted a series of complex degradation mechanisms (see fig 1). The removal of these polymer films is one of the top priorities in conservation science.

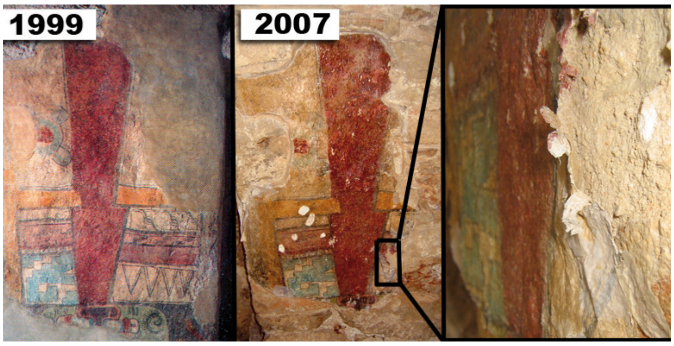


Fig 1. Loss of pictorial layer in a Maya wall painting coated in 1999 with a film of Mowilith DM5.

Nanostructure of cleaning systems

In order to design efficient nanofluids for cleaning artworks, it is necessary to understand their ability to remove given polymer films by determining both their structure and dynamics. Small Angle Neutron Scattering (SANS) is particularly suited for characterising complex nanofluids. NMI3 supported SANS measurements performed on the PAXE instrument of the Laboratoire Léon Brillouin (LLB in Saclay, France) to characterise the structure of two nanofluids (EAPC and XYL).

Structure and kinetics for effectiveness

According to the results obtained we suggest that EAPC interacts with the polymer according to the following model (fig 2):

1. Solvents dissolved in the continuous aqueous phase quickly interact with the polymer coating.
2. A series of exchanges occurs, where solvents migrate from the aqueous phase to the polymer, from the nanodroplets to the aqueous phase and from the nanodroplets to the polymer.
3. The polymer detaches from the substrate, which is now clean, while the nanodroplets get smaller and re-organise their structure due to the outflow of the solvents.

We propose a similar mechanism for the XYL system, with an identical final step, except that the first step of the process is

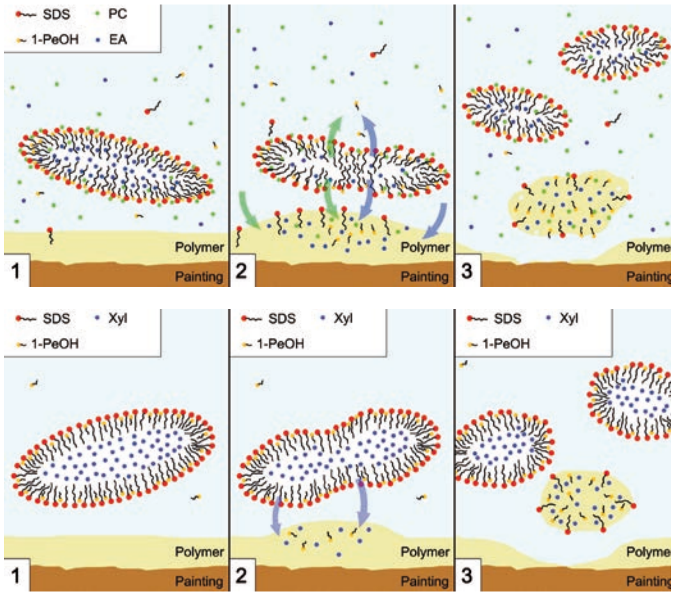


Fig 2. Interaction mechanism between the detergent nanostructured systems (top: EAPC; bottom: XYL) and the polymer coating.

missing, which causes slower reaction speeds. The speed of reaction indeed plays an important role in the effectiveness of these nanofluids in polymer removal from wall paintings during real applications. For an equal duration of application, EAPC is more effective than XYL in removing acrylic coatings.

We believe that a deeper understanding of the nano-structure and the mechanism that lies behind the cleaning process is the key of a more conscious approach to new conservation challenges.

Original publications

M. Baglioni *et al.*, *Langmuir*, 28(43), 15193-202, 2012
M. Baglioni *et al. Nanoscale*, 4, 42-53, 2012
M. Baglioni *et al.*, *Nanoscale*, 2, 9, 1723-1732, 2010
R. Giorgi, *et al.*, *Acc. Chem. Res.*, 43, 695–704, 2010

Michele Baglioni and Debora Berti from the University of Florence, Italy received NMI3 support to perform experiments at LLB.

Healthy diet? Using neutrons to quantify selenium in cereal crops

Health and Agriculture

Selenium (Se) is an essential micronutrient for human health, protecting, for example, against cardiovascular disease, asthma, male sterility and certain forms of cancer. Even though it is a common nutrient e.g. in cereals, it is lacking in the diet of at least 1 billion people around the globe. The few available data indicate that Portugal is one of the countries concerned. For this reason, a research project taking place in Portugal aims to assess the levels of Se in the country's cereals and soils.

Techniques to determine Se in cereal crops

Previous experiments to quantify Se in wheat and rye samples using instrumental neutron activation analysis (INAA) at the Technological and Nuclear Campus (CTN-IST) in Lisbon, Portugal were unsuccessful for the analysed matrices. This time, the team of researchers applied a different approach. The team prepared samples of two wheat varieties – a bread-making wheat and durum wheat – and their respective soils from Elvas (Alentejo province), as well as rye from three Portuguese regions. The samples were then analysed in a slightly modified radiochemical neutron activation analysis (RNAA) at the Nuclear Physics Institute (NPI, Prague, Czech Republic) thanks to NMI3 funding.

While INAA does not provide the necessary sensitivity for those materials, the results revealed that RNAA is indeed a suitable technique for measuring Se in plants and soils. In fact, this technique makes it possible to detect Se even when its concentration is very low.

Se levels in Portuguese cereal crops

Most of the Se was detected in the organic fractions of both plants and soils; the mineral fractions contained reduced or

even undetectable amounts. The only exception to this pattern was the rye straw from Guarda area, in the centre of the country, where the Se value in the mineral fraction was apparently high. Furthermore, the team observed that Se transfer from soil or seed to wheat plants increases as the plants grow through the life cycle.

Se supplements for healthier diets

In the early 80's, sodium selenite was used by livestock breeders for therapeutic purposes. More recently, Finland and the UK have addressed the issue of Se supplements in agricultural crops. In continuation of that work, the results presented here give important insights into Se levels in Portuguese cereals, opening the way to future supplementation trials in the country.

NMI3 thanks Maria do Carmo Freitas and Catarina Galinha from the Nuclear and Technological Institute (ITN - URSN), Portugal, for reviewing this article.

Original Publication

C. Galinha *et al.*, *J. Radioanal. Nucl. Chem.* 294:349–354, 2012

Maria do Carmo Freitas from ITN - URSN and Catarina Galinha from the Technical University of Lisbon in Portugal received NMI3 support to perform experiments at NPI in the Czech Republic.

Neutrons reveal a zone of water increase in soil around plant roots

By A.Morad, UFZ and E.Lehmann, PSI

Agriculture

Water is the main element of the soil-plant-atmosphere system. It is taken up by plant roots at the root-soil interface, and then it is transported to the leaves. How roots take up water from the soil is still not well known. Better understanding of the water uptake mechanism requires new measurement techniques capable of quantifying soil water content in the vicinity of roots with high spatial resolutions.

Neutron tomography setup

It has been so far challenging to measure the water content of the rhizosphere (soil-root interface) around the roots of living plants mainly because it is difficult to measure the content of soil water at distances of less than a millimetre around the roots without interfering with their function. Due to their high sensitivity to hydrous materials, neutron tomography and radiography provide an excellent opportunity to study the distribution of water in soils and roots *in-situ*.

We performed measurements at the Paul Scherrer Institute (PSI) in Switzerland thanks to NMI3 funding. We grew different plant species in aluminium cylinders filled with a sandy soil. We tomographed the samples and monitored the changes in soil water content around the roots as the plant roots took up water and dried the soil. This was done to image temporal and spatial dynamics of water depletion around the roots over a range of soil water contents.

Results

Contrary to models of root water uptake which predict a drier soil close to the roots, we consistently observed that the soil water content close to the roots was higher than far away from the roots (see figure). Given that the roots take up water from the soil, and water can only move from wetter to drier soil, the only explanation is that the soil in the immediate vicinity of the roots has different hydraulic properties than the rest of the soil. It seems that the roots modify the soil in their immediate vicinity towards holding higher water content at the same water potential as the bulk soil. This means that the soil water potential could decrease approaching the root surface. We hypothesise that release of mucilage by the roots into their surrounding soil alters the hydraulic properties of the rhizosphere towards holding higher water contents.

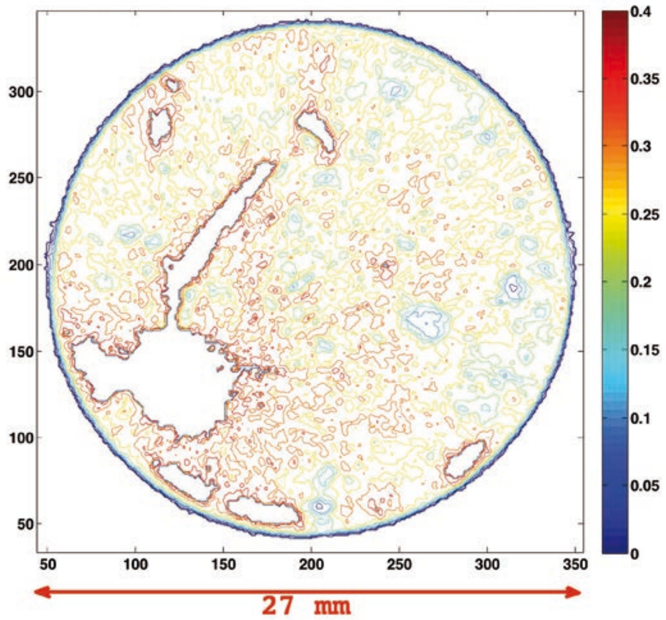


Fig. Micro-scale water distribution around the roots of a plant

Implication of the results

The higher water holding capacity of the rhizosphere helps roots remain hydraulically connected to the bulk soil, ensuring water availability to plants in dry conditions. These findings could help breed plants with high tolerance to drought, and optimise irrigation schedules so that the efficiency of water use could be improved.

Original Publication

A. Moradi *et al.*, *New Phytologist*, 192: 653–663, 2011

Ahmand Moradi and Andrea Carminati from the Helmholtz-Zentrum for Environmental Research, Leipzig, Germany received NMI3 support to perform experiments at PSI.

Characterisation of magnetic fluids for anticancer treatment using neutrons

By M. Avdeev, FLNP, and V. Garamus, HZG

Medicine

Cancer remains one of the most widespread diseases and leading cause of death worldwide. Over the past decade researchers have been investigating the use of colloidal nanoparticles to act as delivery systems for targeted cancer drugs. Magnetic nanoparticles, in particular, have properties that make them good candidates for applications in biomedicine. The transport and concentration of these particles can be controlled by the application of a magnetic field, thus increasing the efficiency of the treatment.

Searching for biocompatible coatings

However, these particles must be designed so that they do not aggregate inside the body because aggregation could provoke complications. To avoid these problems, the particles must be coated with special biocompatible coatings.

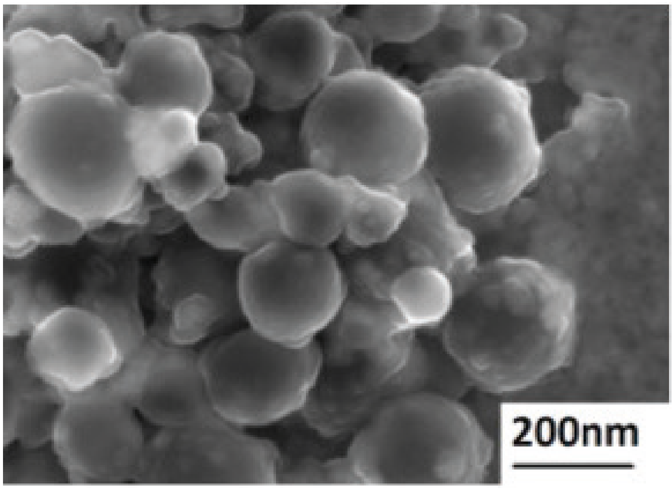


Fig. Magnetic nanoparticles with PEG and drug Taxol encapsulated in a biodegradable polymer

The group of Prof. Peter Kopčansky, from the Institute of Experimental Physics of the Slovak Academy of Sciences, is looking for the ideal compounds and conditions to obtain aqueous suspensions of magnetic nanoparticles, so that they can be coated with drugs and biocompatible components while remaining stable. His group carried out small-angle neutron scattering (SANS) experiments at the Helmholtz Zentrum Gesthaacht (HZG, Germany), thanks to NMI3 funding, to study the coating of magnetite nanoparticles with polyethyleneglycol (PEG), one of the most promising biocompatible polymers (see figure).
As Prof. Kopčansky explains: “Neutron scattering is a unique tool, which allows us to follow in detail the structural changes at the nano-level, after the polymer is incorporated in the system. It finally helps to choose those optimal compositions and conditions, when the aggregation instability is minimal”.

SANS experiments on magnetic fluids

PEG was incorporated into the stabilising shell of magnetite nanoparticles in a water-based magnetic fluid. Our SANS experiments allowed us to see that the addition of large amounts of PEG prompts the development of branched aggregates and a significant decrease in the volume fraction of dispersed magnetite in the system. Our results suggest that PEG is adsorbed in its plain configuration on the magnetite surface, which slightly affects the thickness of the stabilising shell.

Further research to investigate these processes is on-going in collaboration with other institutions.

Original publications

M.V.Avdeev *et al. J. Appl. Cryst.* 46(1), 224-233, 2013
V.Závišová *et al. J. Magn. Magn. Mater.* 323, 1408-1412, 2011
M.V.Avdeev *et al. J. Appl. Cryst*. 43, 959–969, 2010
G.Lancz *et al. Acta Physica Polonica* 118(5), 980-982, 2010

Artem V. Feoktystov from the Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research in Dubna, Russia, received NMI3 support to perform experiments at the Helmholtz-Zentrum Geesthacht.

Proteins perform without water

Life science

The thin film of water around proteins, their hydration water, is vital to the macromolecule's biological activity. It was believed that without hydration water, proteins would not only be incorrectly folded but also lack the conformational flexibility that animates their 3D structures and brings them to life. However, a team of scientists found out otherwise.

Myoglobin behaviour without water

Myoglobin is common to almost all mammals and responsible for the red colour of raw meat. These scientists wanted to assess whether the structure of myoglobin could still move and continue to bind oxygen if all the water was completely removed and replaced by synthetic molecules. By using incoherent neutron scattering at IN16 at the Institut Laue Languevin (ILL, France) and SPHERES at the Jülich Centre for Neutron Scattering (JCNS, Germany), the team was able to monitor the motions in the protein and in the polymer surfactant separately. This separation has been made possible by specific labelling, carried out in a dedicated deuteration laboratory.

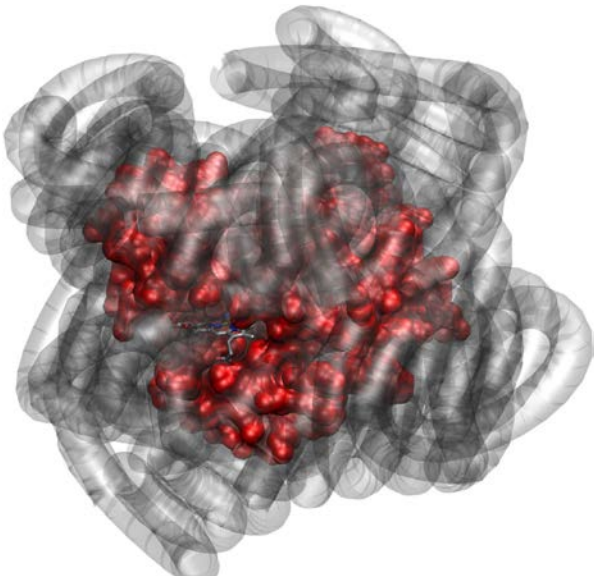


Fig. Myoglobin (red) exhibits biologically relevant dynamics, even when its hydration sphere is replaced by a polymer surfactant corona (grey)

What they found was that the myoglobin molecules surrounded by polymer moved just as well as the wet sample, and that the dry sample had very little mobility. These observations lead to the conclusion that the polymer surfactant coating plasticises protein structures in a similar way to hydration water (see figure).

Knowing that proteins can function outside of water opens them up to use in real life applications because it shows that there are other alternatives if water is unavailable. Examples of where they could be used include biochemical gas sensors and in the development of new wound dressings.

Intrinsically disordered proteins –the tau protein

Now, for the first time, the team has investigated the motions of the tau protein and its hydration shell as representative of IDPs. They wanted to understand how its flexibility and its interactions with water differ from ordered proteins. Combining neutron scattering and protein perdeuteration, they found that the coupling of the tau protein with water motions was much tighter than for folded proteins. They also revealed a greater motional flexibility and more restricted water motions on the IDP surface, as compared to folded proteins. The results provide evidence that protein and hydration-water motions mutually affect and shape each other.

IDPs are of significant interest in a medical context because they can aggregate and cluster together to create the amyloid fibrils behind neuro-degenerative diseases such as Parkinson's and Alzheimer's. Whilst the ordered structure of folded proteins makes it possible to develop drugs that fit into the protein like a key in a lock, the conformational variability of an IDP makes it more difficult. A more in-depth understanding of their dynamics is required and these results are a significant step forward.

This article has been prepared from materials from the JCNS, ILL and PSB. Inside NMI3 thanks Martin Weik for his comments.

Original publications

Gallat F.-X. *et al.*, Biophys J., 103(1), 129–136, 2012

Gallat F. X. *et al.*, J. Am. Chem. Soc., 134, 13168-13171, 2012

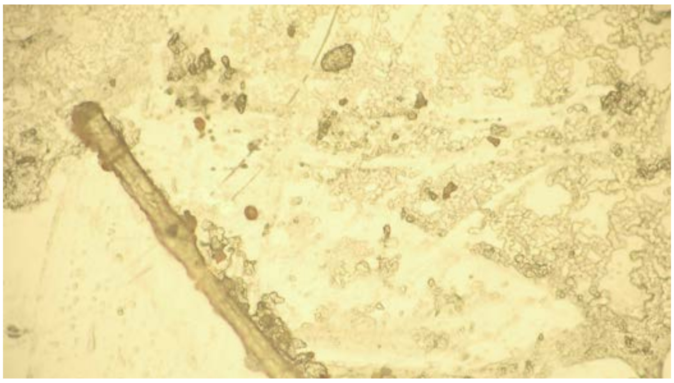
Martin Weik from the Structural Biology Institute and François-Xavier Gallat from ILL received NMI3 support to perform experiments at JCNS.

Assessment of exposure to pollution in industrial workplaces

Indoor air pollution

In industrial settings, employees may be exposed to high concentrations of metals while working indoors. This can cause respiratory symptoms and lung diseases in the short- and long-term. However, the technology imposed by safety regulations to guarantee an acceptable quality of indoor air does not seem to protect against excessive levels of airborne particulate matter (APM).

The analysis of human breath, in the form of exhaled breath condensate (EBC), is a method with potential for measuring individuals' exposure to air pollution, as EBC contains several measurable biomarkers. EBC sampling is particularly suited to workplace assessments, as it is easy to obtain and analyse and is non-invasive for the individual concerned. Further research is necessary however to ensure its reliability as a tool for assessing human exposure to air-borne particles.



Optical micrograph (reflection microscopy) of an EBC sample of a worker, containing particles. Courtesy of IST/ITN

Neutrons give insight into workplace air quality

A team of researchers from Portugal's Nuclear and Technological Institute (IST/ITN) investigated exposure levels for workers in two Portuguese lead-processing factories, by measuring APM levels in the workplace and the EBC of the employees. The team collected APM samples from both factories as well as from a "clean" workplace used as a control. Thanks to NMI3 funding, one of the samples could be analysed by instrumental neutron activation analysis (INAA) at the Higher Education Reactor of TU Delft. The remaining samples were analysed by INAA and by particle-induced X-Ray emission at the IST/ITN's Portuguese Research Reactor. The EBC samples were then

Collection of an EBC sample. Courtesy of IST/ITN

analysed by inductively coupled plasma mass spectrometry (ICP-MS) and were statistically compared, with each other and with the APM samples, so that the potential of EBC as a bio-indicator could be evaluated.

On the way to healthier workplaces

As expected, the results showed significantly higher levels of APM and more exposure biomarkers in the EBC samples (for several metals) than in the outdoor environment and "clean" workplace. Furthermore, the higher APM concentrations corresponded to higher EBC biomarker concentrations, thus demonstrating that the EBC actually reflects exposure to environmental pollution.

These results make an important contribution to establishing EBC as a matrix suitable for use in workplace exposure assessments. EBC sampling could become extremely useful in programmes to control the inhalation of metals in polluted workplace environments. This opens the way to determining the dose inhaled and its effects on the health of the employees exposed. This information will help improve legislation on maximum exposure levels, thus ensuring better protection for workers.

NMI3 thanks Pedro Félix for reviewing this article.

Original publication

Félix PM *et al. Int J Hyg Environ Health. 216(1):17-24, 2013*

Pedro Félix, Marta Almeida and Maria Teresa Pinheiro from ITN received NMI3 support to perform experiments at the Higher Education Reactor of TU Delft.

Neutrons and X-rays help investigate new materials for gas turbines

Transportation

Since the period following the Second World War, the development of gas turbine technology has led to both increased efficiency and higher gas temperatures. It is estimated that future gas turbines will function at temperatures some 200°C higher than those of today. The materials currently in use cannot withstand such high temperatures, and there is now a need to investigate new materials capable of resisting both these very severe temperature conditions and the heavy load on modern gas turbines.

Co-Re-based alloys: a new material for gas turbines

Cobalt-based alloys are routinely used in static components of gas turbines. The group led by Dr Mukherji from the Institute for Materials of the Technical University of Braunschweig in Germany is investigating the structure of cobalt-rhenium-based

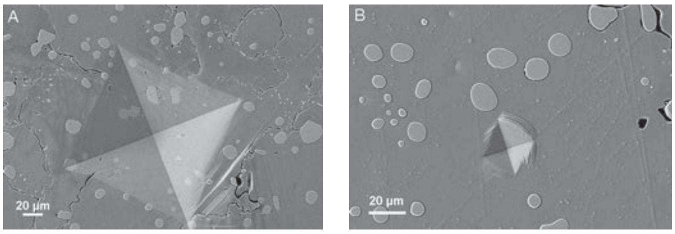


Fig 1. Hardness indentation a) with 10 kg load b) with 300 g load

alloys and their behaviour at high temperatures. These alloys are new for structural applications in gas turbines. By adding rhenium (Re) to cobalt (Co) alloys, it is possible to increase their melting temperature. The group aims to develop alloys whose base metal temperatures can reach 1200˚C.

Neutron and X-ray experiments to characterise structure

Neutron and X-ray techniques provide ideal tools for studying structural changes in materials *in situ* at high temperatures. Dr Mukherji's team has extensively used these tools for characterising Co-Re-Cr alloys. NMI3 has provided support for experiments at the Budapest Neutron Centre (BNC, Hungary) to quantify the boron content in Co-Re-Cr-alloys. Complementary measurements were performed at FRM II and at the Engineering Materials Science Beamline at the Helmholtz-Zentrum Geesthacht outstation at the Deutsches Elektronen-Synchrotron in Germany.

The aim was to investigate the effect of boron doping in Co-Re alloys and the stabilities of the fine tantalum carbide (TaC) precipitates at high temperatures. The group observed that a fine dispersion of TaC precipitates strengthens some Co-Re alloys. These precipitates remain generally stable when exposed to high temperatures.

Looking to the future

Experiments with neutron and synchrotron probes are therefore providing fundamental information in understanding the Co-Re-Cr system. These techniques have helped the researchers observe microstructural involution at high temperatures. Although further research will still be necessary before a technical alloy becomes available for structural applications in turbines, the future looks promising!

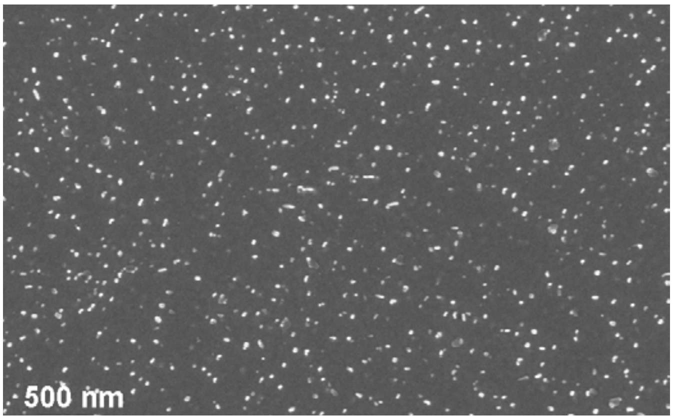


Fig 2. CoRe-2 alloy. Very light dispersion of TaC particles in the microstructure

NMI3 thanks Dr Mukherji for reviewing this article.

Original publications

D. Mukherji *et al.*, *Metall. Mater. Trans. A*, 44 (1) 22-30, 2013
D. Mukherji *et al.*, *Scr. Mater.*, 66, 60-63, 2013

Debashis Mukherji from the Institute for Materials of the Technical University of Braunschweig in Germany received NMI3 support to perform experiments at BNC.

Spins acting like real bar magnets in a new material

Magnetism

The dipolar force between magnetic moments is present in all magnetic systems. The lithium rare earth (RE) tetrafluorides, $LiREF_4$ are an excellent testing ground for the physics of dipolar-coupled systems because the spins in this material behave like real bar magnets. A team of scientists has focused their research on an antiferromagnetic member of the family $LiErF_4$ and investigated the magnetic order, classical phase transition, and transition and fluctuations about the quantum critical point.

Determining the magnetic structure

In order to determine the magnetic structure the team has performed neutron scattering, specific heat, and magnetic susceptibility studies. The NMI3 supported experiments carried out at the Helmholtz-Zentrum Berlin (HZB, Germany). Temperatures down to 0.04°C above absolute zero were achieved so that the team could study the ordered structure and its relevant critical exponents close to both classical and quantum phase transitions. Moreover, very precise heat capacity measurements made it possible to characterise the thermal phase transition to the antiferromagnetic state. Complementary measurements were performed at the Swiss neutron source SINQ at the Paul Scherrer Institute.

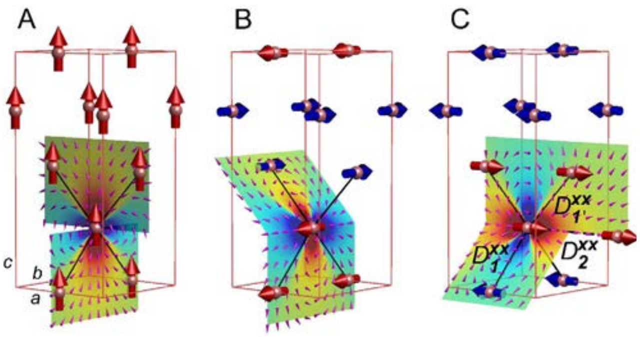


Fig. Magnetic structures of $LiREF_4$. Courtesy of the authors

By using neutron spectroscopy on a single crystal the team has determined the crystal field, which provided the position of the energy levels and the matrix elements of the angular momentum operators. The obtained magnetic Bragg peaks proved that the arrangement of the spins was antiferromagnetic and their intensities were consistent with the bilayered antiferromagnetic structure depicted in the Figure, also verified by powder diffraction. The specific heat showed a pronounced ordering anomaly.

Future implications

$LiErF_4$ has the advantage of a simple, well-characterized Hamiltonian and of being available in large, high-quality single crystals. With the discovery of its properties, researchers now have a material that provides a perfect test bed for getting insights into the fundamental science of quantum dipolar antiferromagnetism.

As Gabriel Aeppli, Director of the London Centre for Nanotechnology, has noted "there are deep connections between what has been achieved here and new types of computers, which also rely on the ability to tune quantum mechanics to solve hard problems" (*in* London Centre for Nanotechnology website).

NMI3 thanks Neda Nikseresht and Henrik Rønnow from the Laboratory of Quantum Magnetism, Switzerland, for reviewing this article.

Original publication

Kraemer C. *et al.*, *Science*, 336 (6087), 1416-1419, 2012

Neda Nikseresht from the Laboratory for Quantum Magnetism of the École Polytechnique Fédérale de Lausanne, Switzerland received NMI3 funding to perform experiments at BER II at HZB.

Investigating a new material for lithium rechargeable batteries

By J. C. Pérez-Flores

Batteries

The existence of the protonated hexatitanate $H_2Ti_6O_{13}$ was only very recently demonstrated, even though only a partial characterisation has been accomplished. Our analysis of data from synchrotron and neutron powder diffraction, combined with IR spectroscopy data, provided us with a precise determination of the crystal structure, thus shedding light on the electrochemical properties of the material and the charge and discharge processes. $H_2Ti_6O_{13}$ finally revealed itself to be an interesting material for rechargeable lithium batteries.

Neutrons: indispensible tools to analyse structure

After synthesising H_2TiO_{13} by Li^+/H^+ ion exchange on $Li_2Ti_6O_{13}$ at mild temperature we used powder X-ray diffraction for a preliminary structural characterisation. We went on to characterise the structure in more detail, using neutron powder diffraction at the Heinz Maier-Leibnitz neutron source (FRM II, Garching, Germany), thanks to NMI3 funding. Additional synchrotron diffraction experiments were performed at the Helmholtz-Zentrum Dresden-Rossendorf outstation in the European Synchrotron Radiation Facility in Grenoble, France. To complete our work, we investigated the lithium insertion/deinsertion processes electrochemically.

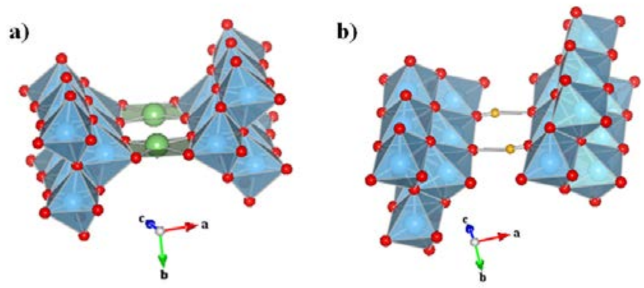


Fig. Schematic representation of the crystal structure of a) $Li_2Ti_6O_{13}$ and b) $H_2Ti_6O_{13}$.

Shedding light on $H_2Ti_6O_{13}$

Whilst X-ray diffraction using synchrotron radiation provides highly accurate phase analysis, neutron diffraction is indispensable for deeper investigations, as both Li and H atoms can be readily located within the structure using subtle intensity changes in the neutron diffraction patterns. We fitted the neutron diffraction data obtained for both parent and proton exchanged derivatives to first refine a structural model without Li or H, respectively. The results suggest that the "skeleton" of this material, $[Ti_6O_{13}]^{-2}$ is preserved during the successive exchange reactions, with very fine changes. For example, $H_2Ti_6O_{13}$ exhibits small shrinking of the a and b axes, while the c axis increases upon ion exchange with protons. The combined but opposite trends in lattice parameters lead to a relatively small decrease in unit cell volume. However, the a and c directions were mainly affected by the Li^+ / H^+ ion exchange due to a change in the tunnel space (see figure).

The properties of $H_2Ti_6O_{13}$ seem to surpass those of the parent compound $Li_2Ti_6O_{13}$. Its reversible capacity is well maintained upon cycling, even at increasing discharge rates. Furthermore, this reversible capacity is similar to that obtained for other titanium oxides already proposed as anode material for lithium rechargeable batteries. We would therefore propose both these materials as candidates for anode material, once their electrochemical performance is optimised.

The future of rechargeable lithium batteries

These results represent a significant step forward, furthering our understanding of the electrochemical behaviour of these materials and confirming their potential in the future development of rechargeable lithium batteries.

Publications

J. C. Pérez-Flores *et al., RSC Advances*, 2(8), 3530-3540, 2012

J. C. Pérez-Flores, A. Kuhn & F. García-Alvarado, *J Power Sources*, 196, 1378–1385, 2011

J. C. Pérez-Flores *et al., Phys. Chem. Chem. Phys.*, 14, 2892–2899, 2012

J. C. Pérez-Flores *et al., Dalton Trans.*, 41, 14633-14642, 2013

Alois Kuhn from the San Pablo University in Madrid, Spain, received NMI3 support to perform experiments at FRM II.

Monte Carlo Simulations and Data Analysis Networks

In NMI3-I, the networking initiatives focused on the Monte Carlo (MC) simulation software, as well as on promoting exchange and collaboration for the development of Data Analysis software.

Software development is of increasing importance for the operation of neutron and muon facilities and involves a large number of people. However, in particular for data analysis software, there is a great deal of 'repetition' – multiple facilities develop code with similar functionalities. For an efficient use of resources, this work package has organised regular networking meetings between developers to:

- ensure widespread exchange of information about developments already underway and
- encourage rationalisation and co-development wherever possible.

Kim Leffman presentation on Monte Carlo Simulations in Garching 2012

Monte Carlo Simulations Network

MC simulation software has been one of the major successes of EU-funded neutron and muon projects through several Framework Programmes (FP). There are two main software packages for neutron simulation experiments, namely McStas (mcstas.org) and VITESS (http://www.helmholtz-berlin.de/ vitess). These are being developed as collaborations across multiple sites in the world and are now an integral part of instrument design. Not only are they used to design and optimise the performance of neutron and muon instruments and components, they are even playing a role in optimising the costs relative to performance, and they will be used for teaching.

Many of the NMI3 Joint Research Activities (JRAs) include tasks that involve writing new sections of code, corresponding to new instrument components being developed. Given that we no longer have a specific JRA devoted to software development, as was the case in NMI3-FP6, these tasks ensure good developer interaction through continued networking.

NaMES: Neutron and Muon European Schools

By Inês Crespo, NMI3 and Ross Stewart, ISIS

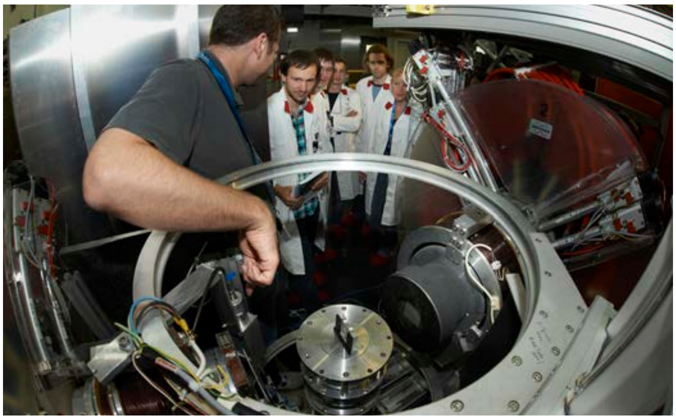
In order to ensure the continued success of neutron and muon research, it is crucial to build future generations of users. On this basis, NMI3 provides funding to schools that address a broad range of topics on neutron scattering and muon spectroscopy, and take place in several countries across Europe.
Since its inception in 2003 and until 2011, NMI3 supported schools that applied for funding through a total of 14 calls for proposals. Philip King from the ISIS pulsed neutron and muon beam source in the UK coordinated this process that included 70 separate awards made and 32 individual schools/workshops supported.

As of 2012, the scope of this initiative slightly changed. It is now called NaMES (Neutron and Muon European Schools) and currently supports a group of 14 selected schools. Laurence Tellier from the Institut Laue Languevin in France and Ross Stewart from ISIS are the coordinators responsible for smoothing the functioning of NaMES.

So far, the feedback from the participants of the NaMES schools has been very positive! In the recently created NMI3 'School series' videos and 'Conversations with the participants' articles, a number of attendees tell about their experiences to help us better understand how neutron and muon schools are helping young researchers in their career development. For further information on topics addressed and dates of forthcoming schools please consult the NMI3 webpages and e-newsletter!

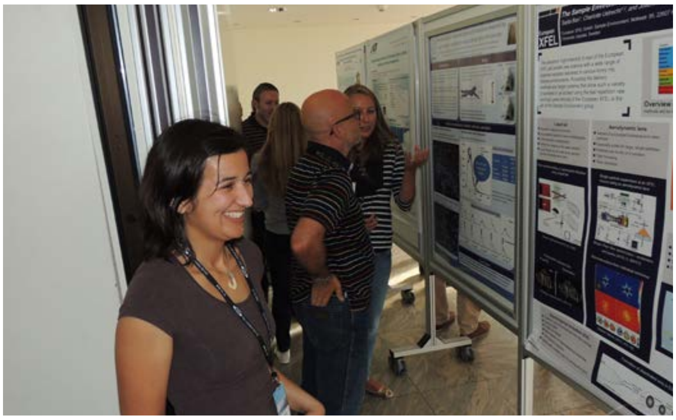
nmi3.eu/about-nmi3/education.html

Students at 2012 ISIS Muon Training School. Photo credits: Stephen Kill FBIPP



Students and instrument scientist at the 2012 JCNS LabCourse. Photo credits: W. Schürmann, TUM.

Students at 2006 Fan du LLB



Poster session at the 2012 PSI summer school. Courtesy of the organisers.

Communicating NMI3

Communication is essential for raising general awareness of the research being carried out in major European centres using neutron scattering and muon spectroscopy. Research with neutrons and muons is providing insight into areas as varied as medicine or the geo-sciences, information technologies, arts and agriculture. NMI3 is increasing the visibility of the work of neutron and muon researchers across Europe, most notably through its website and newsletter and via its presence in the social media.

The NMI3‘s information manager is responsible for these activities. Since the early days of the consortium and until 2010, Ana Claver promoted neutron and muon research through the European Neutron and Muon Portal. Juliette Savin came in to boost our communication activities in 2011, by completely redesigning the NMI3 website and editing the first three issues of the *Inside NMI3* newsletter. Since September 2012, Inês Crespo has been responsible for the NMI3 communication material. This includes the recently implemented e-newsletter, which aims to provide the latest news on European neutron and muon research. Inês also coordinates the upcoming international platform www.neutronsources.org, ensuring the most up-to-date information on neutron research worldwide.

NMI3 will be present with a booth at the European and International Conferences on Neutron Scattering, taking the opportunity to present the results of the Joint Research Activities as well as to inform interested researchers about the NMI3 Access Programme and the Neutron and Muon schools for young researchers. Visitors to our booth will have the opportunity to participate in a fun competition and win special prizes!

We hope you enjoy reading the latest news on neutron and muon research. Don’t forget to inform us of any exciting results, so that we can spread the news!

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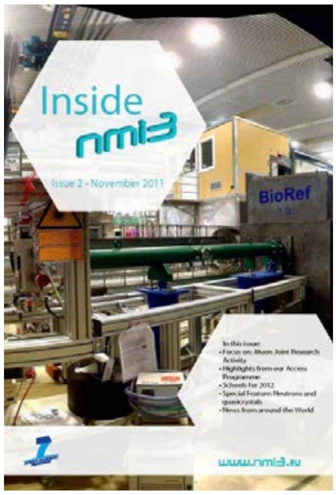

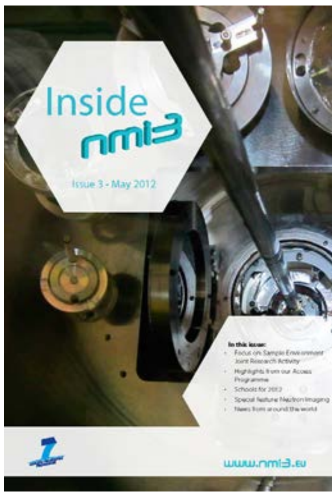

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NMI3 thanks the ILL Translation office for their support.

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