Core of the First Periodic Report over first 18 months

Contents

2.1 *Objectives & work progress & achievements*

WP1 MANAGEMENT & WP2 NETWORKING & WP3 DISSEMINATION

See chapter 1.2.2 Project management

WP4-15 TRANSNATIONAL ACCESS ACTIVITY

See chapter 2.3 Access Activity

WP16 MONTE CARLO SIMULATION AND DATA ANALYSIS NETWORKING

Objectives

Software development is a key aspect of the operation of neutron/muon facilities and is of increasing importance. However, there is a great deal of „repetition" – development of different code, but with similar functionality, in multiple places. This is not an efficient use of resources. This work package will organise regular networking meetings between developers to (a) ensure widespread exchange of information about developments already underway and (b) encourage rationalisation and co-development wherever possible.

Work progress

a. Monte Carlo Simulation meeting in Alpe d'Huez (F) March 17th, 2010

b. Data analysis meeting in Abingdon (UK), May 3rd, 2010-08-12

Achievements

a. The meeting between simulator experts has improved the already good collaboration between simulator groups. It was agreed that the simulator groups would continue to share ideas for development and validation of simulation packages. As a particular focus point, polarized neutrons was selected. The collaboration has arranged a common training course in May 2010 and will arrange an international workshop as a satellite to the ECNS in Prague 2011.

b. Deliverable 16.02. The data analysis meeting, as documented in the meeting report, has led to an improved common understanding of ongoing data analysis developments among NMI3 partners. It has also raised awareness of the need for greater collaboration, of potential projects which might form a focus, and of 'good practice' for software development. This was confirmed at the 'heads of facilities' meeting at GKSS in June 2010.

WP17 NEUTRON OPTICS

Objectives

During the late 80' and early 90', tremendous improvements have been made in the fabrication of neutron mirrors. These new coatings allow building guide systems with an increased neutron flux of a factor 3 to 4. More recently these improved super-mirrors have been implemented into optical devices: trumpet guides, ballistic guides, polarizing benders etc. and have permitted to improve existing spectrometers. Our challenge is now to go some steps further and to increase the luminosity of the neutron spectrometers even more. We think that the neutron optics technology and components, which are presently available, enable to design new spectrometers which can be at least 10 times brighter than existing ones. The principles that will be demonstrated could easily be implemented at other facilities. The outcome will be a more efficient use of the existing neutron sources. This would benefit directly in the short term to neutron users.

We propose to focus on 3 main objectives: (i) High flux reflectometry, (ii) High flux SANS and (iii) Focussing of thermal neutrons. Each thematic task gathers instrument scientists who are experts in their fields (reflectometry, SANS, diffraction or imaging) and who have a direct interest in improving their spectrometers. Most of the proposed developments should eventually be implemented on existing spectrometers in the short term. The implementation of these innovative technical solutions will require technical developments which will in general benefit to several tasks.

Most of the optics developments require advanced numerical simulations. Monte-Carlo simulation programs will be upgraded or rewritten to include new advanced components and optimization tools. This will also benefit to a wide community.

The Workpackage 17 *Neutron Optics* is divided into 4 main tasks:

Work progress

Task 17.2: High flux reflectometry and energy analysis

Task 17.2.1a: High flux reflectometry using focussing optics

The initial project was based on the REFOCUS concept[1]. This concept has been upgraded so as to simplify its implementation. A new scheme allows to split the monochromatization and focussing functions which provides more flexibility to the design together with a much easier implementation. The new design has been baptized SELENE. A detailed technical report of the new SELEN design can be found on the Neutron Optics Website [2]-[3]. A prototype SELENE bench is to be implemented at the PSI for early 2011 (scale ½).

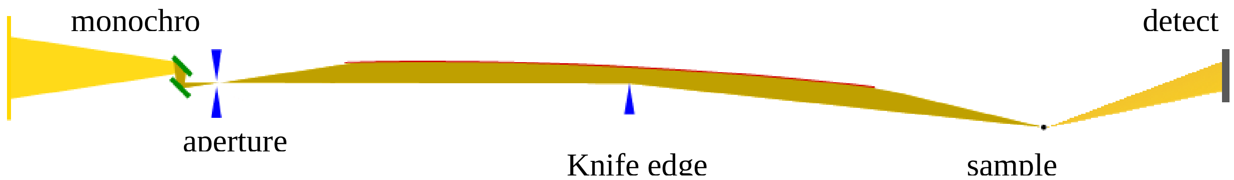


Figure 1: SELENE design (J. Stahn)

[1] F. Ott and A. Menelle, NIM A **586** (2008) 23–30. REFOCUS: A new concept for a very high flux neutron reflectometer.

[2] J. Stahn, NOP 2010 Conference

[3] "Study on a focusing, low-background neutron delivery system", J. Stahn, T. Panzner, U. Filges, C. Marcelot, P. Böni, Nuclear Instruments and Methods A, doi: 10.1016/j.nima.2010.06.221

A new McSTAS component has been developed at PSI in order to model the new spectrometer. It allows in particular to take into account: (see Figure 2)

– true curvature

– all surfaces with individual properties

– individual shapes

– neutrons can pass by

– nesting of devices

The implementation of off-specular scattering is under way.

The new McStas component has been submitted to the McStas library.

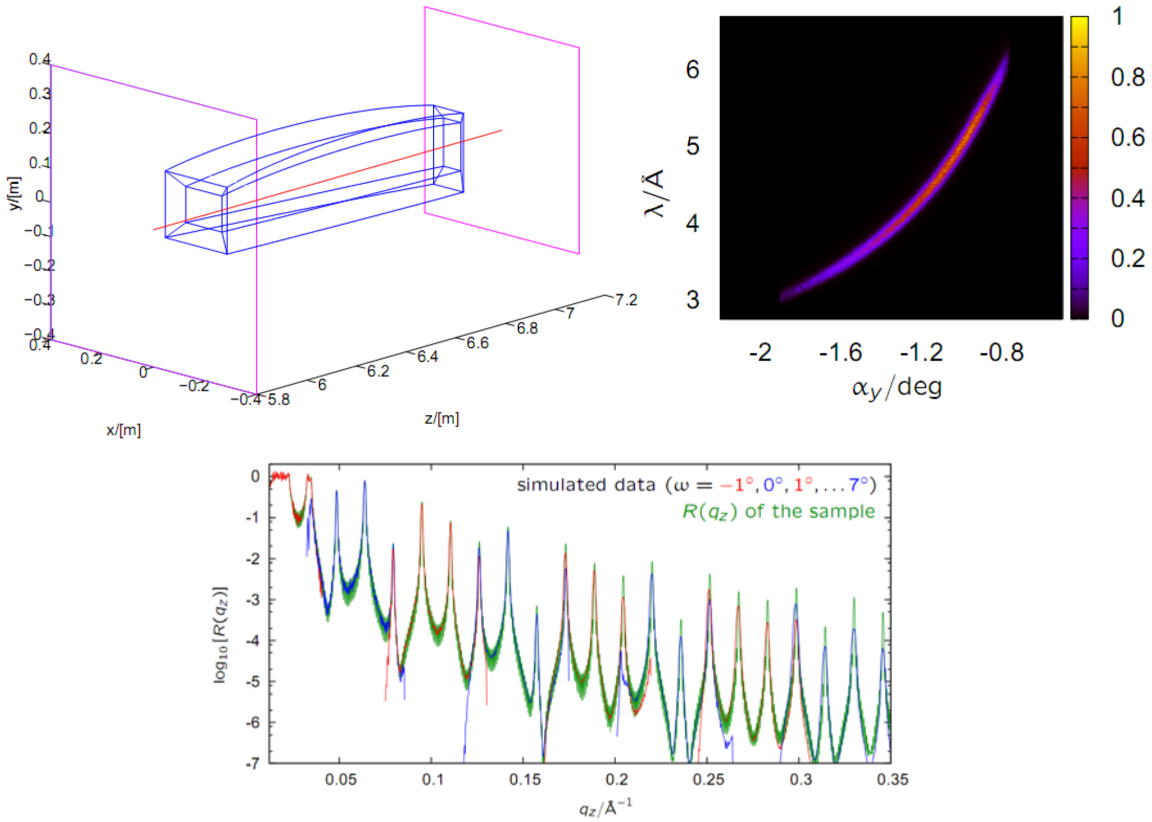


Figure 2: (a) New McStas component. (b) Monte-Carlo simulation of the SELENE set-up. (c) Expected reflectivity measured on a multilayer using a SELENE set-up.

Task 17.2.1b: Compact Energy Analyzer

The compact energy analyzer will be using mutltilayer monochromator deposited on silicon substrates. Construction of a first prototype shall start in 2010. It will be limited to wavelengths longer than 0.4nm. The problem of the diffuse scattering will be assessed. The coatings are to be deposited at the PSI. The mirrors are to be assembled at HZB.

A presentation of the device has been made during the NOP'2010 conference[4]

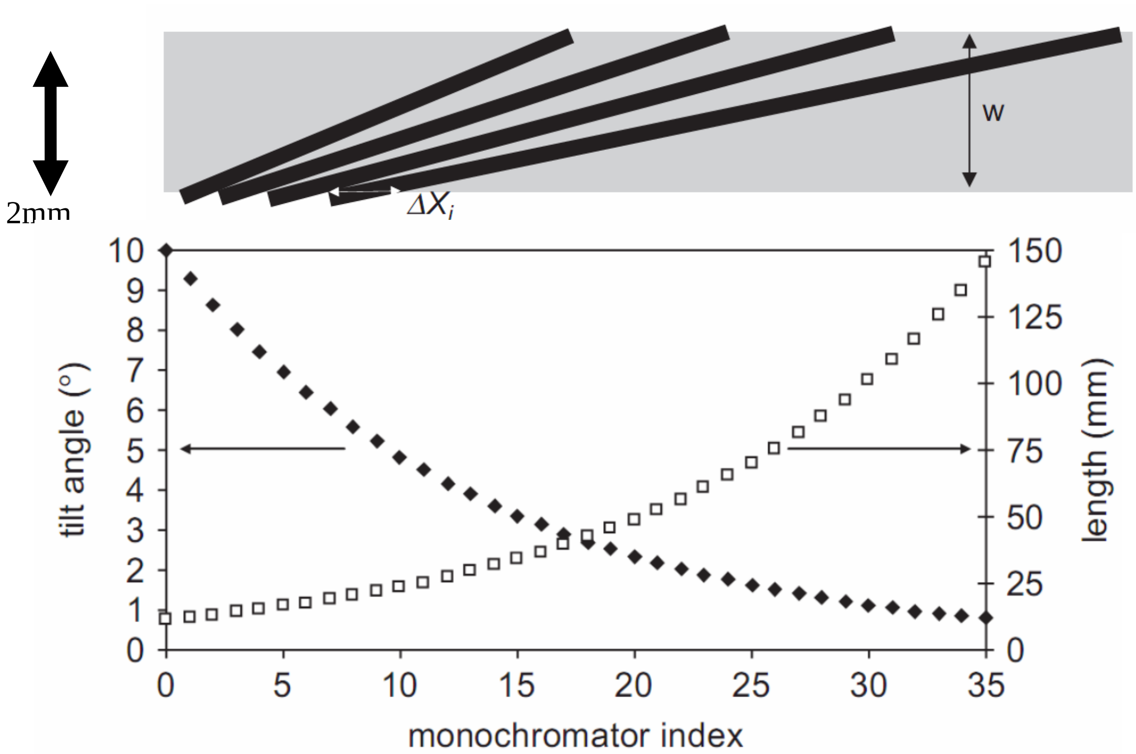


Figure 3: Principle of the compact energy analyzer. (a) Sketch of the super-mirror positions. (b) Parameters of the different mirrors (tilt angle and length of the energy analyzer.

Task 17.2.2: Refraction-encoded reflectometry

Up to the present we have had only two methods to measure the neutrons' wavelength, monochromation via crystals or a selector and time-of-flight (TOF). Both approaches are extremely wasteful with ~99% of neutrons being thrown away contributing nothing more than noise. Ideally we would like to have a detector that told us not just the intensity at a given position but the wavelength too. With such a device ILL machines would have the same useful flux as the ESS as both sources would have approximately the same mean intensity.

We are all familiar with the refraction of white light into its component colours on traversing a glass prism. Neutrons have the same property and this process can be used to measure the wavelength with the only loss being in the absorption of the prism material[5]. Indeed the gain in using this method is the ratio of prism transmission to that of the chopper which can be 10-100x depending on the resolution.

A large MgF_2 crystal (100mm long) has been tested at the ILL on the D17 spectrometer in order to build an energy dispersive spectrometer. It has been shown that data of similar quality can be obtained compared to the ToF technique.

[4] F. Ott, NOP Conference

[5] Cubitt R. Nucl. Inst. And Methods 558 547-550 (2006)

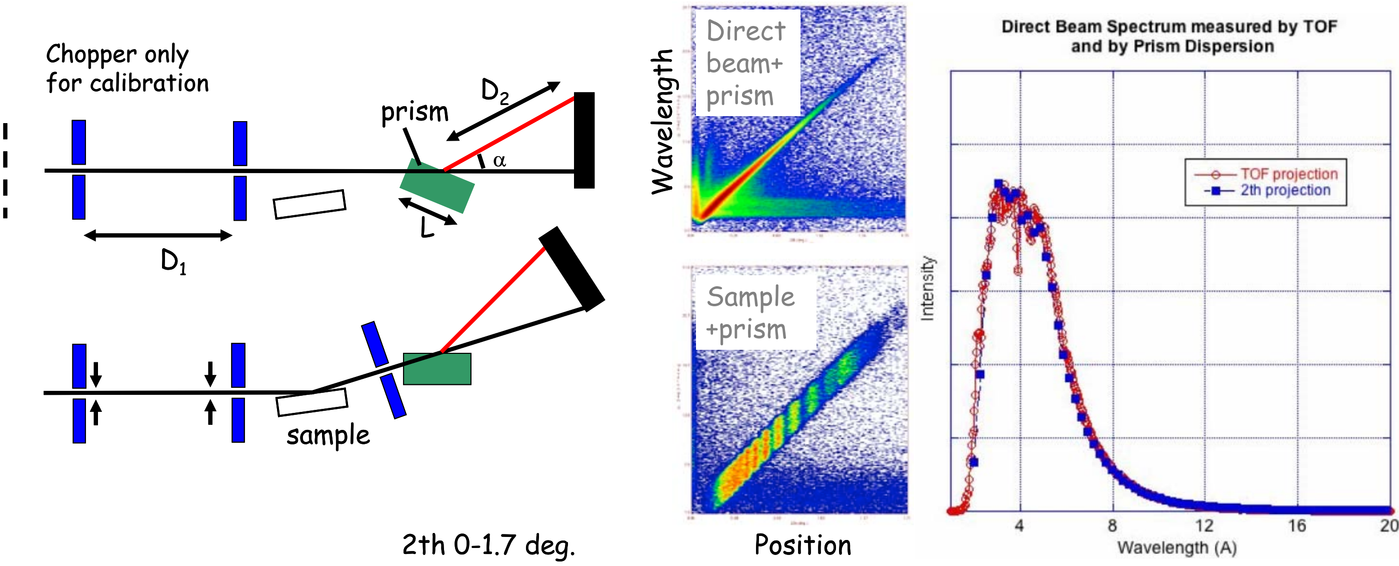


Figure 4: (top) Reflectivity measurement using the ToF method (used for calibration) followed by a measurement using refraction through a crystal. (bottom) Comparison between the ToF measurement and the refraction measurement. (R. Cubitt, D17, ILL)

The present limitation is due to the lack of very high resolution efficient neutron detectors. This can be overcome by setting a standard detector at a large distance (>6m). To have a reasonable resolution the experiment was carried out on the AMOR reflectometer at PSI (**Figure 5**). The main reason for this was the longer sample to detector distance available over ILL machines. There is no need to have a complex prism shape. In this case a very flat single surface of MgF_2 was used. The experiment was quite simple. First, in standard TOF mode the main beam was measured through the prism enabling a calibration of the deflection as a function of wavelength. Then the chopper was stopped open and the intensity measured again, this time with a gain of ~30x in intensity. A sample was introduced before the prism and the reflected beam was passed through the prism at the same angle (Figure 6).

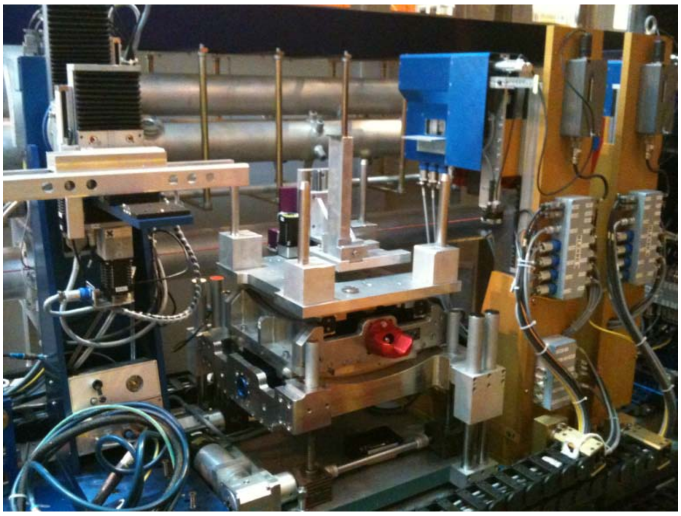


Figure 5: The AMOR reflectometer at PSI showing the sample in the centre and prism on the left.

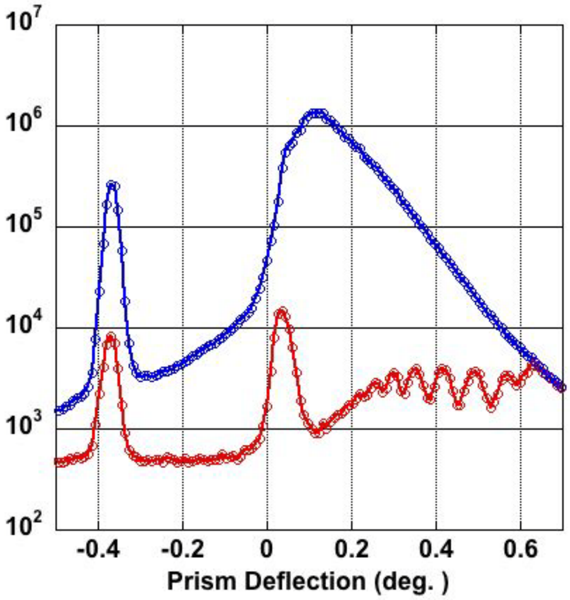


Figure 6: The main beam (blue) and reflection (red) after passing through the prism. The peak on the left is the reflection from the prism surface and the central peak is beam that missed the prism. To the right of this peak the different wavelengths are dispersed at different angles on the detector.

Reflectivity was produced by simply dividing the two data sets after the subtraction of the appropriate background (Figure 7). For comparison, a measurement at approximately the same resolution of 10% measured with the standard TOF method is shown in Figure 7 but ten times the measurement time was required to produce the same quality data.

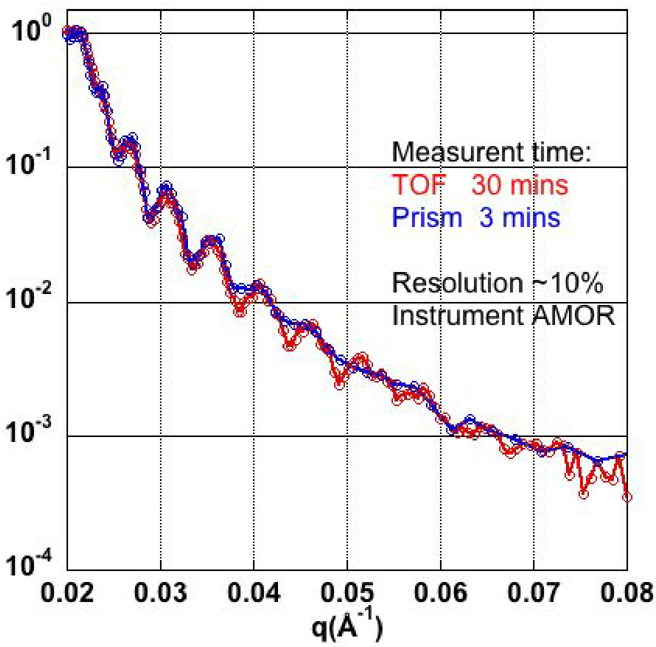


Figure 7: Reflectivity measured by the prism method (blue) and TOF (red). It was not possible to have the same resolution as a function of wavelength as AMOR operates with a constant dλ/λ like D17 and

FIGARO in this case set at 10%. The prism produces a resolution with constant dλ which varies from ~5% at 12Å, corresponding to the lowest q and ~20% at 2Å at the highest q. The sample was a 1200 Å layer of Nickel on glass.

With better detector resolution (here the detector was 5m away with 2.4 mm resolution) 5% wavelength resolution is possible even at 2A where a gain of ~100x would be possible. A reflectometer at the ILL with a long enough detector distance (~10 m) and a resolution < 1 mm would be capable of measuring a factor of 15 in q and a reflectivity less than 10^{-4} in sub-second timescales thus opening up a new area of fast kinetic studies. Such a machine, which would also be naturally disposed for GISANS measurements, will be proposed as part of the ILLs' future suite of instruments.

Composite MgF_2 prisms have been fabricated and tested at HZB. To check the applicability of MgF_2 prisms as an energy analysing device, the deflection, reflectivity and attenuation of a MgF_2 single crystal with a prism shaped structure has been measured.

The sample used for the measurements consists of a 50mm x 20mm x 2mm MgF_2 single crystal block. The upper 0.5mm of the material are cut into the shape of 33 prisms with an angle of 45° to the basis. Each prism deflects the beam by $\Theta = 0.00225°$, so the deflection by the prism array is expected to be $\Theta_{defl} = 0.074°$. Experimentally a value of 0.081° was determined.

An attenuation coefficient of $\mu=0.030cm^{-1}$ was found for this material. The same transmission rate was measured when the beam passes the prism array. Because in this case there were in average only 25mm MgF_2 in the beam path, the value of the attenuation coefficient is $\mu=0.055cm^{-1}$. This is about 1.8 times higher than expected.

The angular width of the neutron beam increases from 0.014° by passing the pure MgF_2 by 0.005° and by passing through the prisms by 0.015°.

The increase of the beam width and the high intensity losses while the beam passes through the prism array indicates that the prisms surfaces are very rough and the neutrons are diffusely scattered. Due to the high deflection power of this material, the MgF_2 prism array is still a good candidate for an energy analysing device. The diffuse scattering can be reduced by polishing the surfaces to increase the angular and wavelength resolution.

Task 17.2.3: Wavelength encoding by Bragg diffraction

The objective of this task is to develop an energy dispersive device based on diffractive optics.

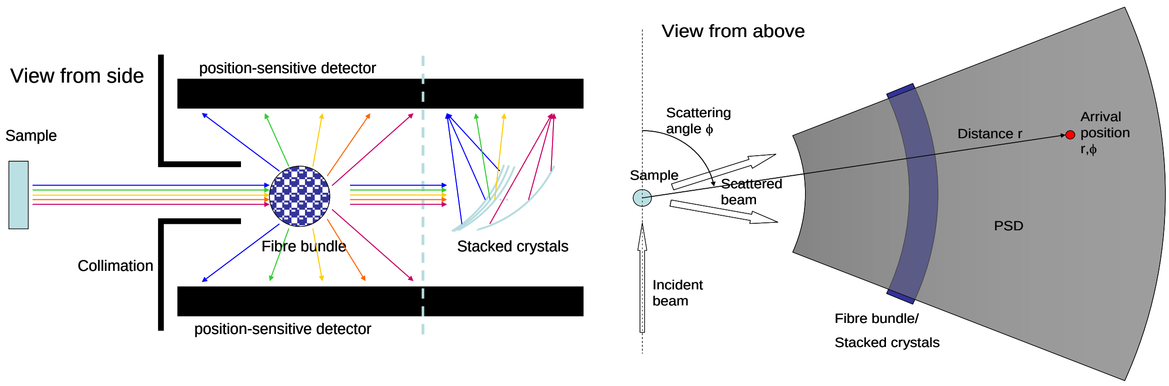


Figure 8: Principle of an energy dispersive device based on diffractive optics.

Dispersive monochromators based on multiple reflection (P. Mikula and J. Saroun)

Another objective of this task is developing of dispersive monochromators based on multiple reflection (namely double reflection) processes which can be strongly excited in bent perfect crystals and thus provide very high angular and wavelength resolution, simultaneously. In some cases the wavelength resolution can approach the resolution of the backscattering device, however, realized on a conventional neutron scattering performance. Jan Saroun has developed new algorithm within the RESTRAX program (ver. 6.0.8) permitting MC simulations of these double reflection processes. After testing several crystal slabs of different orientations, many strong double reflection processes has been identified at λ in the vicinity of 0.16 nm and after that new high-resolution diffractometer employing multiple reflection monochromator and operating at λ = 0.16 nm has been built in NPI Rez.

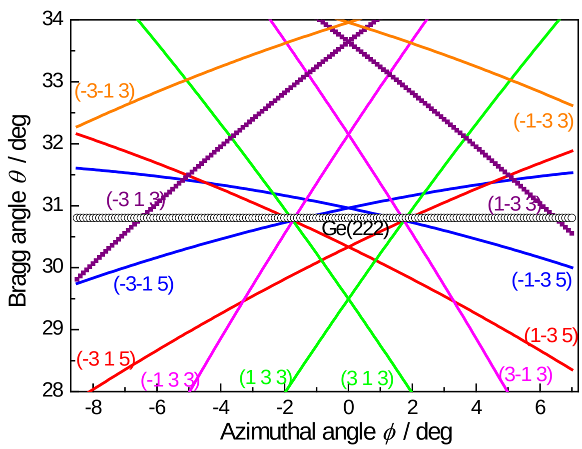


Figure 9: Azimuth-Bragg angle map for double reflection occurrences related to the 222 forbidden reflection in diamond structure. Φ = 0° corresponds to the position of the crystal slab with the main face parallel to the 112 planes and perpendicular to the scattering plane. θ =30.8° is the mean Bragg angle for Ge(222) forbidden reflection at the fixed wavelength of λ=0.1657 nm

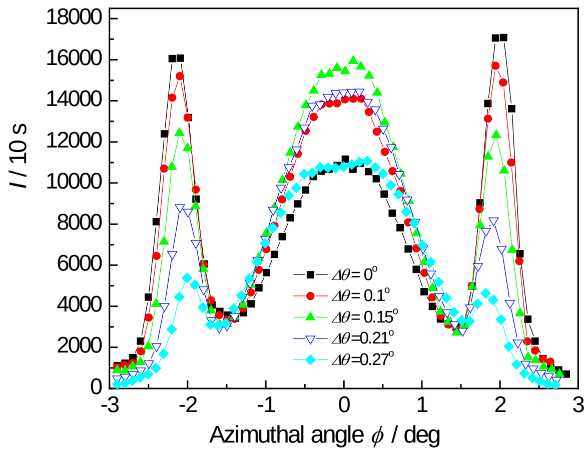


Figure 10: Intensity versus azimuthal angle dependence for Ge(222) bent crystal slab (the thickness t = 4 mm and bendingb radius *R*=9 m) having the main face parallel to the (112) plane for different $\Delta\theta$ from the mean Bragg angle of θ =30.8°. Symmetric transmission of Ge(222) in the arrangement: bent perfect Si(111) crystal (premonochromator) + bent Ge(222) crystal was used.

J. Šaroun, P. Mikula, J. Kulda, *Monte Carlo simulations of parasitic and multiple reflections in elastically bent perfect single-crystals*, In the Proc. of Int. Workshop on Neutron Optics NOP2010, Alpe d'Huez near Grenoble, France, 17-19th of March 2010, Nucl. Instrum. Methods, in print.

P. Mikula, M. Vrána, J. Šaroun, B.S. Seong, V. Em and M.K. Moon, *Multiple neutron Bragg reflections in single crystals should not be considered negligible*, In the Proc. of Int. Workshop on Neutron Optics NOP2010, Alpe d'Huez near Grenoble, France, 17-19th of March 2010, Nucl. Instrum. Methods, in print.

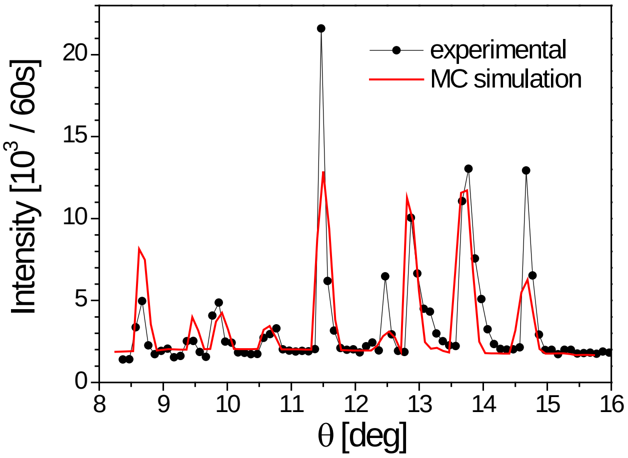


Figure 11: θ-2θ scan of the bent perfect Si(111) crystal set in symmetric transmission geometry. Four double reflections contribute to the peak at θ=11.5°: 313/404, 044/133, 133/022, 202/313.

Task 17.3: Advanced Focusing Techniques

Task 17.3.1: Multichannel focusing guide

Phil Bentley has developed genetic algorithms applied to the optimisation of neutron optics. The programs are available @http://philbentley.com/

Genetic algorithms have shown that is was possible to design focussing guide which were 30% more efficient than human designed guides.

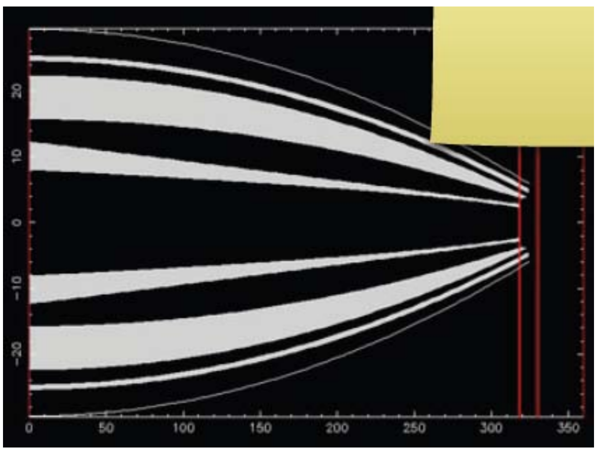


Figure 12: Multichannel focussing guide optimized using genetic algorithms (P. Bentley, J. Appl. Cryst. 42 (2009) 217.)

Task 17.3.2: Adaptive Optics for extreme Environments

The McStas component (Guide_four_side.comp) developed within task 17.2.1 has been successfully used to simulate adaptive optics and benchmarked with the existing component (Guide_tapering.comp) used for the simulation of parabolic and elliptic guides. The neutron optics of a parabolic focusing system has been modelled using the new component.

Extensive Monte-Carlo simulations have been performed using Guide_tapering.comp to explore the limits of focusing using elliptic focusing guide systems. It is shown that in combination with apertures focal spots with a diameter of approximately 0.1 mm can be produced (Figure 13). For stronger focusing and larger focal lengths, Montel-mirrors are more favourable. In a future project the performance of Montel-mirrors and nested devices (Wolters) may be evaluated and compared with conventional focusing systems.

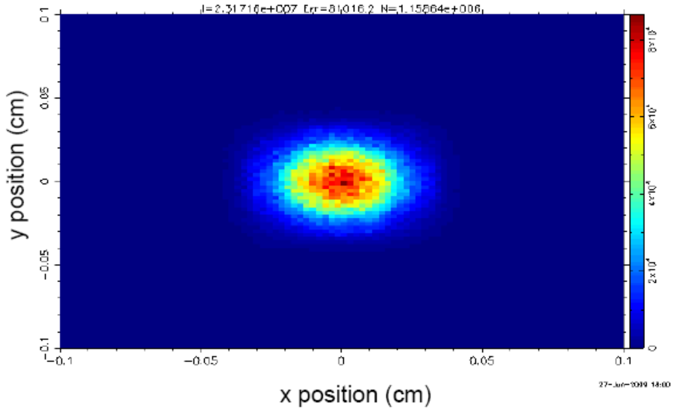


Figure 13: Intensity distribution at the focal position of an elliptic guide. An aperture with a diameter of 1 mm is inserted directly after the exit of the guide (R. Valicu, Workshop on Neutron Delivery Systems, ILL, 2009).

Monte-Carlo simulations have been performed to study the focusing properties of a parabolic mirror using the McStas component Guide_four_side.comp. Based on the results, a full scale adjustable focusing device has been built (Figure 14a). The focal length of the parabola is defined by the movement *x*. The position of the focal point transverse to the optical axis is adjusted by means of the rotation angle α (Figure 14b).

a)

b)

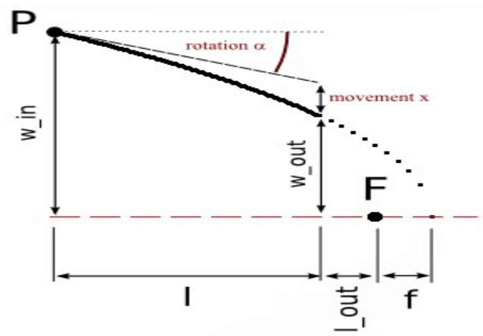


Figure 14: : a) Prototype of an adjustable focusing device using a mechanical bending mechanism. b) Defining parameters of the parabolic focusing device. The parameters to define the parabola are the rotation angle α and the movement *x*.

The performance of the device was tested using the beam line Morpheus at PSI. Figure 15a shows the deflection angle 2θ of the neutron beam versus the rotation angle α. To show that the intensity in Figure 15a is not only an ordinary reflected beam, the device was shifted for every reasonable 2θ -α combination perpendicular to the beam and a detector scan was performed. Only for the correct focal point the maximum of the intensity stays at the same detector position (reflected beam will be shifted). Figure 15b-d show detector scans for 3 different 2θ -α combinations. It is clearly visible that Figure 15c (α = 0.6 deg) yields a real focal point. The results prove that adaptive focusing works.

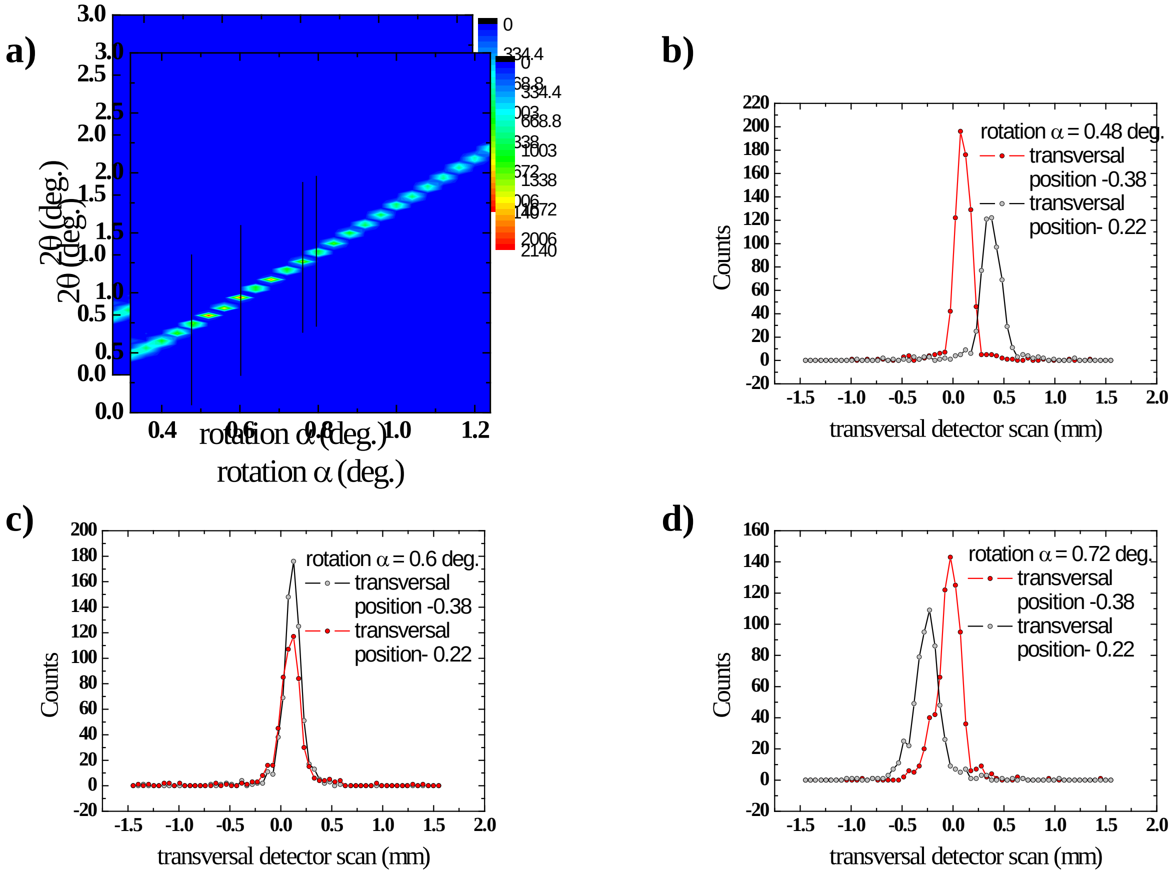


Figure 15: a) Deflection angle of the neutron beam versus α. b)-d) determination of the focal point by transverse detector scans for selected 2θ -α combinations. b) and d) are only reflected beams, c) corresponds to a real focal point.

The experimental results agree well with the numerical simulations. A detailed report of the system has been given during the NOP conference[6]. Further simulations shown that by increasing the critical angle of reflection up to m = 6, significant gains in flux can be realised (Figure 16).

Presently, designs are developed to integrate the bending mechanism into a focusing lens system. The first step is a parabolically curved mirror with a five point bending mechanism, which one can be quickly extended to a guide by adding a second identically designed mirror.

The project on adaptive optics proceeds as expected according to the official gant chart. The Monte-Carlo simulations for the test device have been conducted and a test device has

[6] R. Valicu, NOP 2010 Conference, Oral presentation; M. Schneider, NOP2010 Conference Poster presentation.

already been designed and built. Ahead of the schedule, first neutron measurements on the test device have been performed and analysed. Presently, a full scale device for applications is being designed. The final design is due by Feb. 2011.

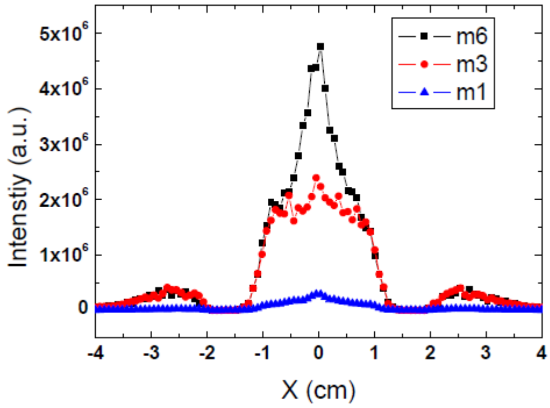


Figure 16: Gain in flux at the sample position for coatings *m* = 1, 3, and 6

Task 17.3.3: High resolution imaging using reflective optics

In a first task we propose to demonstrate by means of Monte-Carlo calculations that elliptic neutron guides lead only to minor distortions of the phase space and can thus be efficiently implemented for neutron radiography and tomography. In a second task we would like to develop focusing devices using a nested Wolter-type mirror system and advanced supermirror technology to produce focal spots with a diameter of the order of 0.1 mm. The emerging beam can be used as a bright neutron source for a cone beam geometry allowing to increase the resolution and at the same time magnify the object, similarly as it is done with x-rays from micro-focus tubes. This way, the limited spatial resolution of present day neutron detectors may not limit radiographies anymore.

Simulations (D 17.3.3.1, D 17.3.3.2)

Two focusing neutron guides (linear taper and elliptic) and a straight neutron guide with circular pinhole (for comparison) each of total length 3 m were simulated using the Monte Carlo simulation code McStas[[7]]. During the course of the simulation, cold neutrons were supplied by a curved neutron guide (cross section: 30 mm × 120 mm, length: 20 m, radius of curvature 3000 m) with a coating of ^{58}Ni, which gives 1.2 times the critical angle θ_c of natural Ni (m=1.2). A flight path of 5 m between the end of the secondary guide (straight, linear taper and elliptic) and the detector plane represents the length of the real instrument, Fig. 1a. The intensity distribution measured at the detector position (Fig. 1a) shows that the elliptic guide provides an almost homogeneously illuminated area of approximately 20 cm × 20 cm. The linearly tapered guide illuminates a similar area as the elliptic guide, but with a less uniform radial intensity distribution. The standard (straight guide with circular pinhole)

[7] K. Lefmann and K. Nielsen, Neutron News **10/3**, 20 (1999).

configuration provides a beam that is just 1/9 the area of the beams produced by the focusing guides.
The simulated intensities at the detector position for a defined *L*/D ratio are depicted in Fig. 1b. In order to simulate different *L*/*D* ratios, circular pinholes with various diameters *D* were placed at the exit of the guide system for the straight and linear taper setups and at the focal point of the elliptic guide. The distance between the exit of the guide and the detector plane was kept constant at L = 5 m.
The comparison shows that the neutron flux in the central part of the beam depends only on the *L*/*D* ratio but not on the neutron guide configuration (Figure 17b). A study of the spectral homogeneity shows i) that for the elliptic set-up the spectrum is essentially uniform, ii) that transmitted by the linear tapered guide is almost uniform, except far away from the beam axis, while iii) for the straight guide the spectrum softens rapidly towards the edges (Figure 17c). The enlarged beam cross-section and improved spectral and intensity homogeneity of the elliptic guide are expected to lead to an improved performance in real applications.

Experiment (D 17.3.3.2, D 17.3.3.3)
An elliptic guide was tested experimentally and results were compared with those obtained using a straight guide. The set-up used a focusing elliptic neutron guide with a length of 500 mm, a rectangular cross sections of 10.6×21.2 mm^2 (entrance) and 4×8 mm^2 (exit) and a supermirror coating m=3. The focal points were at a distance of F_1=1580 mm and F_2=80 mm from the exit of the guide. Note that these values are different from those used for the simulations in Fig. 1b. Experiments were performed at CONRAD, the neutron imaging beamline at the Hahn-Meitner-Reactor of the HZB [8]. The beam was characterised at F_2 using a cold neutron spectrum (maximum at 3 Å). To allow a comparison with the

[8] A. Hilger et al, Physica B **385-386**, 1213 (2006).

[25] http://www.swissneutronics.ch/fileadmin/download/snag_newsletter_2009-december.pdf

conventional geometry, gain factor images with and without the focusing guide were recorded.
Using the elliptic guide the width of the focal point in the central area of the beam was found to be 0.36 mm in the horizontal and 0.55 mm in the vertical direction (Figure 18). The spot size was determined using Gaussian fits of the horizontal and vertical intensity profiles through the focal point. The focused white neutron beam shows a maximal intensity gain of 80 at the focal point (compared to the straight guide). The small size of the focal point is a good precondition for the realisation of a point source geometry with a high *L*/*D* ratio.
Use of the elliptic guide discussed above allowed enlargement of the beam dimensions by a factor of 3 at a distance of 5 m from the end of the guide to the detector at CONRAD, thus enabling tomographic investigations of large samples. Additionally, the small focal point provides a good *L*/*D* ratio, which is important for achieving high spatial resolution – particularly concerning experiments involving samples that cannot be placed close to the detector plane.

This configuration has been used to investigate a particle filter for a diesel engine (15 cm diameter) at a distance of 4.2 m between the focal point (80 mm from the guide exit) and the detector plane. 600 projections of the sample were recorded at equidistant angular steps with a total rotation of 360°, and the data were reconstructed using an algorithm for cone-beam geometry (Figure 19a left). A measurement using a straight guide and a circular pinhole with D = 2 cm and identical data collection parameters was also performed; the data were reconstructed using a filtered back-projection algorithm assuming parallel-beam geometry (Figure 19a right). In this case the sample had to be scanned through the beam in order to illuminate it completely since the sample was larger than the beam cross-section.

The possibility for magnification provided by the cone-beam set-up was studied by visualizing a periodic grid (Gd mask deposited on Si wafer) with a periodicity of 1 mm. The measurement at 1.2 m distance from the detector shows a magnification of 20 % (right hand side of Figure 19b).

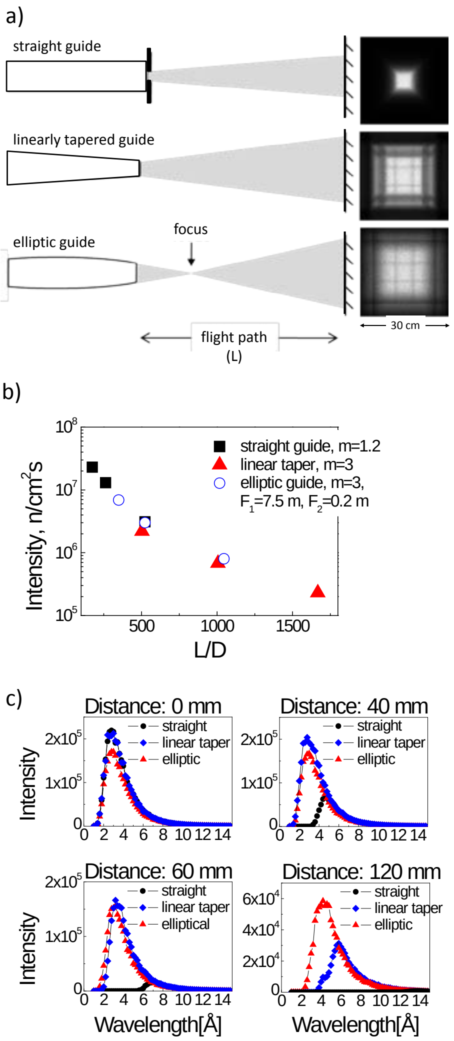


Figure 17: Monte Carlo simulations of different neutron guide configurations. (a) Intensity distribution 5 m behind the guide exit in a detector plane of 30 cm × 30 cm for a straight guide **with a pinhole of 1 cm;** linearly tapered guide **(coating m=3.0, length: 3 m, entrance: 3 cm × 3 cm, exit: 1 cm × 1 cm);** elliptic guide **(coating m=3.0, length: 3 m, entrance: 3 cm × 3 cm, exit: 0.89 cm × 0.89 cm, F_1=7.5 m, F_2=0.2 m). (b) Neutron flux integrated over the central area of the detector (1 cm × 1 cm) as a function of *L/D* . (c) Spectra calculated at different distances from the beam axis integrated over an area of 1 cm × 1 cm.**

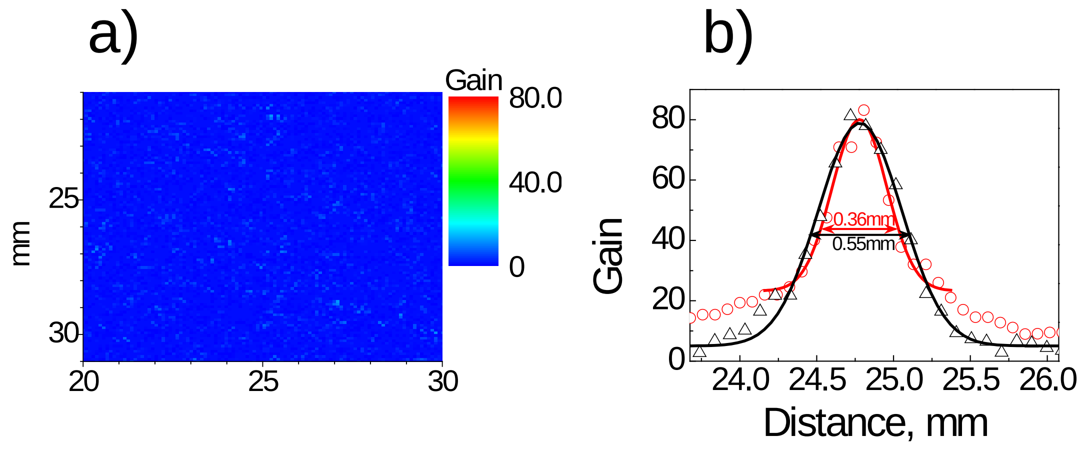


Figure 18: Characterisation of the beam at the focal point of the elliptic guide. (a) Intensity distribution. (b) Horizontal (○) and vertical (Δ) intensity profiles were fitted by Gaussian functions.

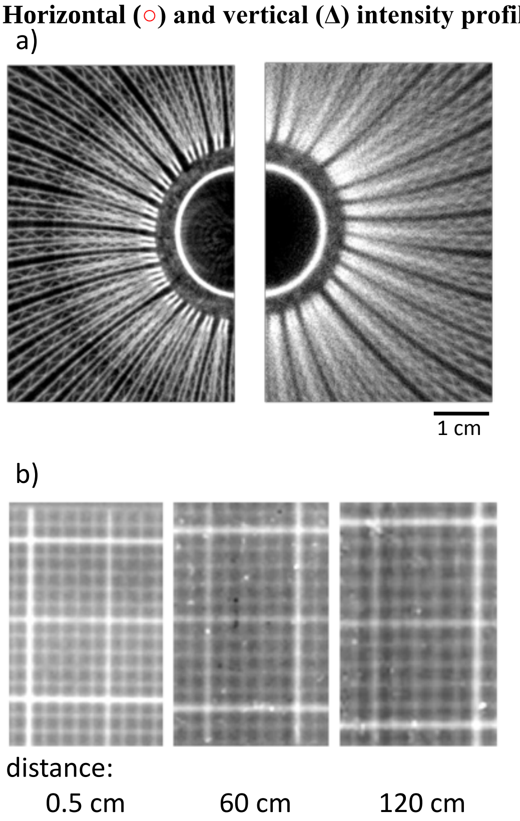


Figure 19: Imaging experiments. (a) Tomographic slice of the central part of a particle filter measured in the cone-beam geometry (left) and parallel-beam scanning geometry (right). (b) Magnification of a grid with 1 mm periodicity measured at different distances from the detector (0.5 cm, 60 cm and 120 cm) in the cone-beam geometry.

[25] http://www.swissneutronics.ch/fileadmin/download/snag_newsletter_2009-december.pdf

Task 17.3.4: Focussing SANS

Task 17.3.4a: Focussing SANS using reflective optics

We propose a new concept of neutron focalisation on SANS spectrometers using a combination of curved super mirrors (SM). The aim is to design a focusing system which is achromatic and has no absorption. The proposed design combines advanced neutron optical element such as parabolic and elliptic SM. Figure 20 presents the device design. A parabolic SM focuses the beam from the exit of the guide to make it a point source at its focal point *Fp*. An elliptic SM with its primary focal point (*Fe1*) lying at the same position as *Fp* images *Fe1* to its secondary focal point *Fe2* according to the properties of ellipses. Now, if a sample is placed after the elliptic SM and a detector is located at *Fe2*, then we build a focusing system with working on reflection (around 85% for m=3 SM) and achromatic. Therefore, SANS instruments could benefit of this technique in terms of flux at the sample.

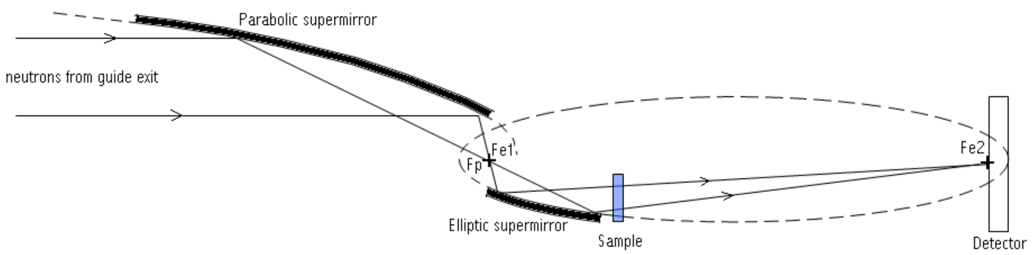


Figure 20: Design of the focusing device with a combination of parabolic and elliptic supermirrors

This task is presently in its modelling phase. The question of the provider of the curved mirrors is under discussion.

Task 17.3.4b: Focussing SANS using refractive optics

Aspherical lenses have been successfully tested at JCNS.

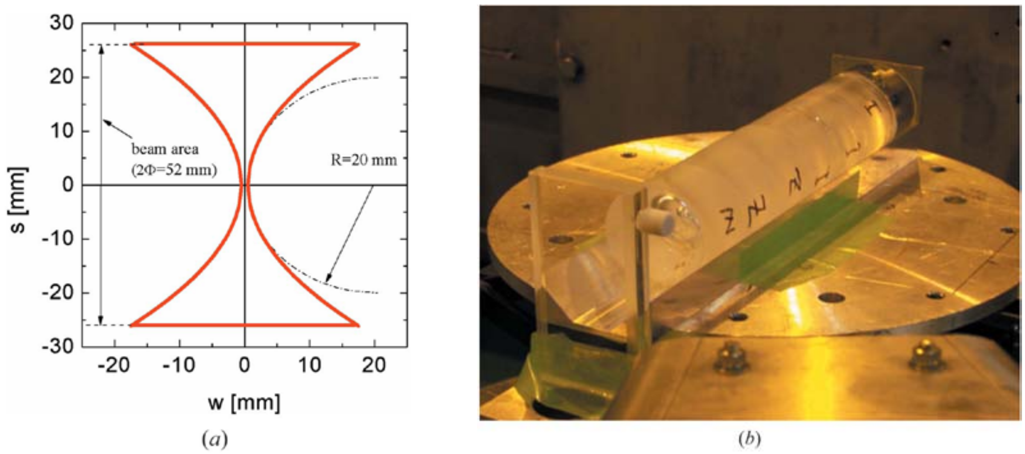


Figure 21: (a) Design of the aspherical MgF2 lens with an inner radius of 2 cm and a 5.2 cm diameter for the neutron beam area. (b) Photograph of an array of aspherical MgF2 lenses.

The resolution determining elements of a focusing SANS instrument have been determined by analytical theory and computer simulations. The coefficients of each contribution were determined by both methods. At present, we have done the calculations for radially averaged scattering in Gaussian approximation. This state of description corresponds to a focusing SANS which enhances the intensity, but not necessarily the resolution. Astonishingly, the contribution of gravitation is rather weak for this approach, while all other contributions were already well estimated by Mildner. From the present approach it becomes clear, that gravitation and the lens diameter are important for high resolution experiments. Furthermore, higher order corrections need to be taken into account (Figure 22). This is the immediate task to be taken next.

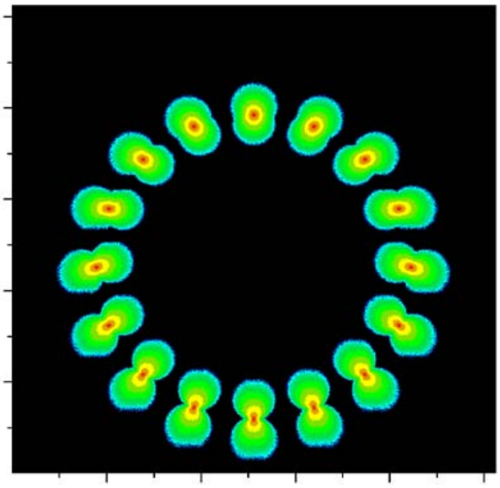


Figure 22: : Resolution functions of a gravity influenced focusing SANS instrument. The distinct peanuts arise from 'Bragg-reflexes' given by the simulation, and present a resolution function at this point.

For intensity optimized focusing SANS without high resolution, we solved tasks 17.3.4.5 – 17.3.4.6 without limitations, and the residual tasks (17.3.4.7 and 17.3.4.8) will be easily fulfilled with existing software. The high resolution option needs higher order terms apart from a Gaussian description, which bears some difficulties. Simulation-wise tasks 17.3.4.5 and 17.3.4.6 are fulfilled, but we need a proper (and simple) analytical description. So we stay within the schedule.

Task 17.3.4c: Beam shaping for SANS

Neutron guide system for multiple beam SANS have been modelled at BNC. The different designs are based on the initial suggestion by A.Wiedenmann, R. Gähler and K. Anderson (Multiple Beam SANS (http://www.sns.gov/workshops/Long_Pulse/LPSS_SANS.pdf).

A detailed report has been presented during the NOP2010 conference.

Details about the different investigated designs can be found on the Neutron Optics website.

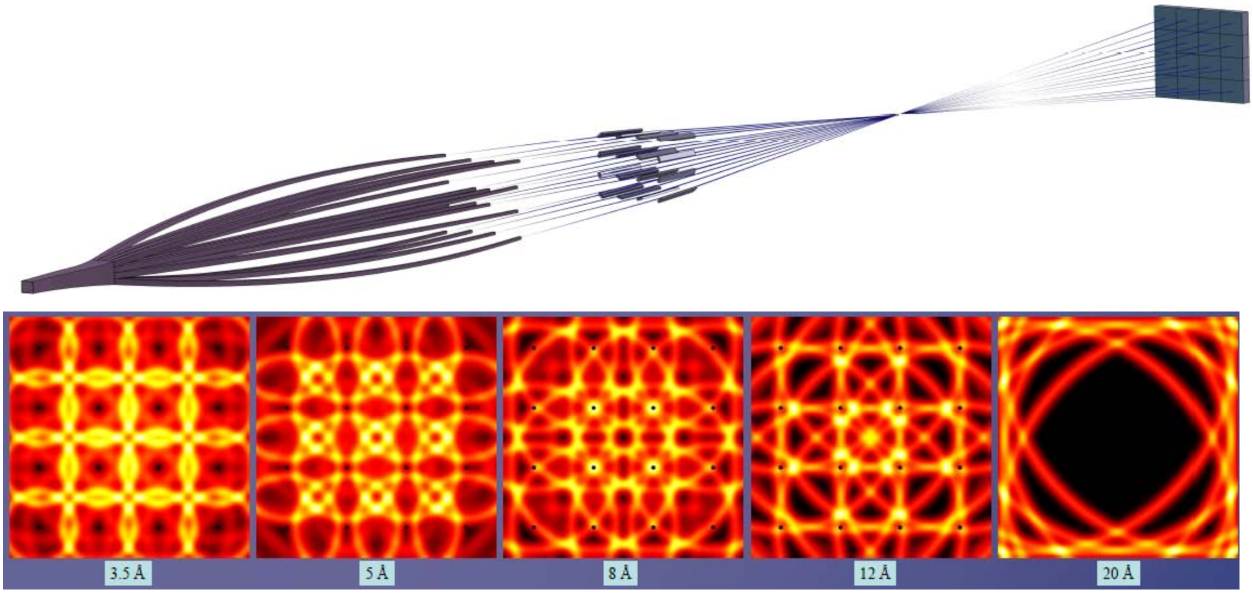


Figure 23: (a) Example of one of the multiple beam shaping design; (b) Different scattering pattern obtained for different wavelengths.

Task 17.4: Monte-Carlo simulations of complex optics

Task 17.4.1: Modelling of interacting optical elements

A first solution has been proposed to handle assembly of basic optical elements to build a new McStas component. The technique has been demonstrated on a “meta-component” including a guide with an embedded, wedged, polarizing mirror system of the HZB type. A publication on this technique is under preparation.

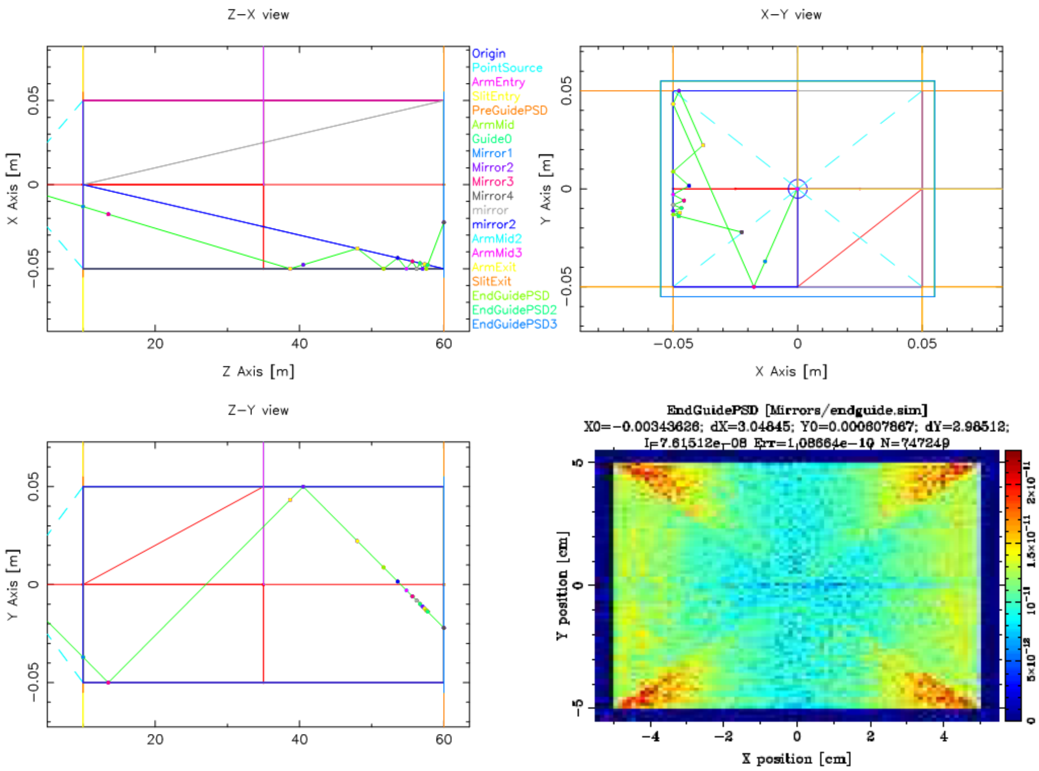


Figure 24: (top) Axis-parallel visualisation of single neutron ray travelling through single-mirror guide with inserted wedge mirrors. Notice reflection on guide wall, inserted wedge, guide wall, and transmission through inserted wedge. (Guide 50 m long for visualisation purposes.); (bottom-right) Transmission through the system.

A presentation describing the technique is available on the Neutron Optics Website.

Task 17.4.2: Optical simulation work bench

A McStas/VITESS school has been been organized in May in Ven, organized by Peter Willendrup, Linda Udby, Klaus Lieutenant, and Emmanuel Farhi (see www.essworkshop.org)

Another workshop, for more specialized use of McStas will be organized in 2011.

Achievements WP17

In most of the Tasks of WP17 Neutron Optics, the first 18 months objectives were to develop refined designs of the initially proposed devices together with modelling tools. This phase is now over and actual prototypes are presently being built. During the next 18 months, experimental characterization of the devices will be performed.

Task	Description / Major progress	Partner
Task 17.2	High flux reflectometry and energy analysis	
Task 17.2.1a	REFOCUS: A new concept for a very high flux reflectometer	CEA
	The design has been upgraded and simplified using the SELENE concept which splits the monochromatization and the focussing optics. Monte-Carlo simulations of a final design	

	have been performed.	
Task 17.2.1b	Compact Energy Analyzer	CEA
	The design of the first prototype is completed. The coatings will be made at PSI. The device will be assembled at HZB	
Task 17.2.2	Refraction-encoded reflectometry	ILL-HZB
	A large MgF2 prism has been delivered. The first refraction tests have been performed on D17 and AMOR demonstrate that the principle is working.	
Task 17.2.3	Wavelength-encoding by Bragg diffraction	ILL-NPI
	Monte-Carlo simulations of multi-analyzer system in transmission arrangement have been performed using SimRes at NPI	
Task 17.3	Advanced Focusing Techniques	
Task 17.3.1	Multichannel focusing guide	ILL
	Monte Carlo simulation component for multi-channel guide have been performed	
Task 17.3.2	Adaptive Optics for extreme Environments	TUM
	MC-simulations have been performed. A test device has been fabricated and its performances have been characterized. The performances of the demonstrator are fully satisfactory.	
Task 17.3.3	High resolution imaging using reflective optics	HMI
	Monte-Carlo simulations have been performed. A first demonstration measurement has been performed showing that the principle of image magnification works very well when using elliptic guides. The first results are published N. Kardjilov et al, J. Appl. Phys. 108 (2010) 034905	
Task 17.3.4	High flux focussing SANS	
Task 17.3.4a	Focussing SANS using reflective optics	CEA
	The demonstration set-up is designed. A decision needs to be made on who will proceed to the actual fabrication of the device	
Task 17.3.2b	Focussing SANS using refractive optics	FZJ
	Aspherical lenses are available at JCNS and the first tests have been performed. Detailed numerical modelling has been performed	
Task 17.3.3c	Beam shaping for SANS	BNC
	Different designs of multibeam SANS set-up have been evaluated by Monte-Carlo simulations	
Task 17.4	Monte-Carlo Simulation of complex optics	
Task 17.4.1	Multichannel focusing guide	DTU
	A first solution has been proposed to handle assembly of basic optical elements to build a new McStas component. The technique has been demonstrated on meta-component including a guide with an embedded, wedged, polarizing mirror system of the HZB type. A publication on this technique is under preparation.	
Task 17.4.2	Optical simulation workbench	DTU
	A McStas/VITESS school has been organized in May in Ven, organized by Peter Willendrup, Linda Udby, Klaus Lieutenant, and Emmanuel Farhi (see www.essworkshop.org)	

WP18 DEUTERATION

Objectives

This JRA will provide the next methodological quantum leap for 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. NMI3 will widen the access of neutron scattering methods to biologists throughout the EU, both by extending the range of problems that can be tackled, and by reducing the cost impact of sample preparation. It will exploit an obvious synergy with the NMR (Nuclear Magnetic Resonance) community, which also has important needs for isotope labelling and within which there is increasing use of neutron scattering. Hence the involvement of NMR scientists at the partner institutes (eg Watts at Oxford/ISIS, Sattler at TUM/FRM-II, Blackledge at IBS/PSB) in this JRA is highly significant.

Work progress

18.2: Deuterated biomass

Sub Task 18.2.1: Identification of suitable biomass systems (D18.2.1 complete)

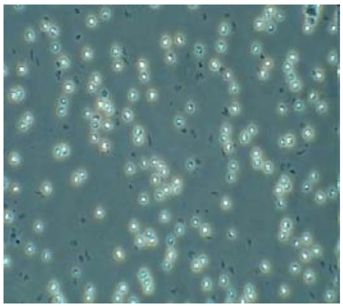
Two different algae species *Chlorella sorokiniana* and *Chlorococcum littorale* have been tested for their capacity to be used as organisms for the production of deuterated biomass. The deuterated biomass will be used for the isolation of deuterated precursors (nucleosides from DNA, amino acids from proteins) and for the development of complex growth media (*H. salinarium).*

We contacted the Culture Collection of Algae and Protozoa, SAMS Research Services Ltd.Dunstaffnage Marine Laboratory, Dunbeg, UK to obtain a culture of *Chlorella sorokiniana* (CCAP 211/8K), but it turned out that their culture was contaminated with fungi. We finally obtained an identical strain from the SAG Culture Collection in Göttingen, Germany (SAG 211-8k *Chlorella sorokiniana*). This single-celled fresh water micro algae reproduces at an extremely fast rate, renewing into four new cells in every 17 to 24 hours. It is known for its high content of chlorophyll, (highest compared to any known plant). The culture temperature of this algae is 37°C-40°C with an pH optimum of 6.7, max. specific growth rate: $0.27h^{-1}$, volumetric productivity of 0.5 g dw L-1 h^{-1}.

The strain *Chlorococcum littorale* (NBRC 102761) has the phenotype high CO_2 tolerant, growth to high density in cultures. The strain has been isolated from sea water in Japan (Kamaishi Bay, Pacific Ocean, its optimal growth temperature is 18°C. The strain has been obtained through the Resource Collection Division NITE Biological Resource Center (NBRC, Chiba, Japan).

Chlorella sorokiniana was identified as the best system for this type of biomass production.

Sub Task 18.2.2: Biomass growth conditions in H media (in progress, due to complete end of month 24)



Report so far: Flask cultures in H media are now being tested. *Chlorococcum littorale* was grown in BG11/Volvox medium 4:1 at 2% CO_2. For *Chlorella sorokiniana* (see inset picture) it was first necessary to isolate single colonies on BG11 agar plates at 37°C. Colonies appeared after 15 days. Then 2ml of BG11 medium were inoculated with one colony. The doubling time for *Chlorococcum littorale* was much longer than for *Chlorella sorokiniana*, reinforcing the choice of *Chlorella sorokiniana* for the optimisation of growth conditions in H media. Photobioreactor (see picture below) protocol development is also under way.

18.3: Labelling of Pichia Pastoris

Sub Task 18.3.1: Identification of suitable expression systems (D18.3.1 complete)

Report:

Following substantive tests, we have chosen 2 model expression systems: one for secreted human serum albumin (HSA) from Invitrogen, and one for secreted hen egg lysozyme developed in the Dlab. We developed perdeuterated minimal media allowing growth of *P.pastoris* as well as expression of recombinant proteins in *P.pastoris.* Then protocols for adaptation of *P.pastoris* to growth in deuterated minimal medium were developed and small scale expression for the 2 model systems carried out. Refinement of protocols for cost-effective perdeuteration has been started. Later on we will develop protocols for "match-out deuteration" in Pichia

Sub Task 18.3.2: Pichia expression in H media (in progress - nearly complete, due to finish at end of month 24)

Report so far: Extensive expression tests were carried out using hydrogenated media, yielding a protocol that is summarised below:

Growth medium

BSM medium pH 6 (Tomida et al 2003):

H_3PO_4, 26.7 ml L^{-1}, $MgSO_4.7H_2O$, 0.93g L^{-1}, KOH, (4.13g L^{-1} glycerol),

40mL L^{-1} and 4.35ml L^{-1} PTM1 trace salts

PTM1 trace salts per L:

$CuSO_4.5H_2O$, 6 g , NaI, 0,08 g , $MnSO_4.H_2O$, 3 g , $Na_2MoO_4.2H_2O$, 0.2 g , H_3BO_3, 0.02 g , $CoCl_2$, 0.5 g , $ZnCl_2$, 20 g , $FeSO_4.7H_2O$, 65 g , biotin, 0,2 g , H_2SO_4, 0,5 mL

BSM flash evaporated and the powder taken up

40g L^{-1} of glycerol added as carbon source

5g L^{-1} of methanol added

Results for both HSA and lysozyme were tested by mass spectrometry and (in the case of lysozyme) by crystallisation and X-ray crystallographic measurements. Both confirmed the fidelity of the expression systems and their suitability for deuterium labelling work as part of the next phase of the project.

Publications/dissemination

Publications

Zhu, X., Ng, S.Y., Gupta, A.N., Ho, B., Egelhaaf, S.U., Forsyth, V.T., Haertlein, M., Moulin, M., Van der Maarl, J.R.C., *Phys. Rev. E* 81 (6), 061905 (2010).

Vijaykrishnan, S., Kelly, S.M., Callow, P., Bhella, D., Forsyth, V.T., Byron, O., Lindsay, J.G., Solution structure and characterisation of the human pyruvate dehydrogenase complex core assembly, *J. Mol. Biol.* 399, 71–93 (2010).

Taylor, J. E., Callow, P., Swiderska, A. & Kneale, G. G. Journal of Molecular Biology (2010) 398, 391-399.

M.J. Clarke, J.B. Artero, M.J. Moulin, P. Callow, J.A. Carver, P.C. Griffiths, M. Haertlein, J.J. Harding, K.M. Meek, P. Timmins, J. Regini, Biochimica et Biophysica Acta (2009).

Paciaroni A, Cornicchi E, Marconi M, Orecchini A, Petrillo C, Haertlein M, Moulin M, Sacchetti F. J. R. Soc. Interface (2009) 6, 635-640.

Isabelle Petit-Haertlein, Matthew P. Blakeley, Eduardo Howard, Isabelle Hazemann, Andre Mitschler, Michael Haertlein and Alberto Podjarny, Acta Cryst. (2009). F65, 406–409.

Conferences/workshops

Sept 2010	EPSAM Fest, Keele University, UK.
Sept 2010	2020 Vision Millennium Symposium, World Trade Centre, Grenoble, France.
August 2010	*Bio-interfaces: From molecular understanding to application*, Lund University, Sweden
June 2010	Structural Glycoscience: Methods and Instrumentation, ESRF Grenoble
October 2009	*Neutrons in Biology Symposium*, Santa Fe, New Mexico, USA
October 2009	Trends and Perspectives in Neutron Scattering on Soft Matter, Tutzing, Germany
June 2009	*Neutrons in Biology*, Lund University, Sweden
May 2009	Nottingham University, UK, as part of the BeNatural consortium
Mar 2009	Paul-Scherrer Institute (PSI), Villigen, Switzerland,
Jan 2009	Copenhagen University, Denmark

Task 18.4: Segmental labeling

Task 18.4.1.1: Model system design

We have established one model system for segmental labelling, which consists of the tandem RNA recognition motif domains (RRM1-RRM2=RRM12) of human splicing factor U2AF65. This system is considered most useful, as we have established high yield standard expression in *E.coli* and numerous biochemical, NMR, SAS and structural data are available for the two domain protein (Figure 25). The two domains interact only weakly in solution. As it is expected that the ligation efficiency during expressed protein ligation will depend on how strong the two domains interact we are investigating two additional multi-RRM proteins where the two domains that should be ligated interact to different extents, i.e. strong or not at all, to be able to evaluate the segmental labeling efficiency and optimize protocols for such systems.

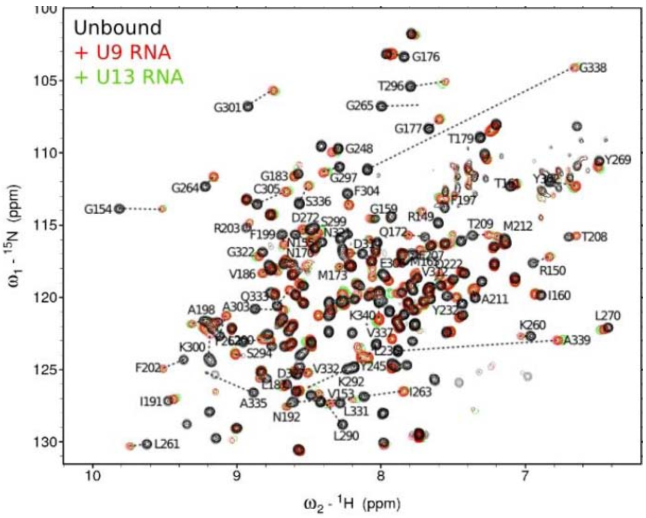


Figure 25: NMR spectra of U2AF65 RRM12 free and when bound to U9 or U13 RNA oligonucleotides. The tandem RRM domains serve as a model system with (weakly) interacting domains for ligation. The three-dimensional structures are known (Simon et al, Angew. Chem. 2010; Mackereth et al, submitted) and numerous NMR and SAS data exist.

Task 18.4.2.1: Protein expression

We have obtained expression vectors for *in vivo* and *in vitro* protein ligation and performed initial text expression of protein domains/fragments for segmental labeling. We are testing and optimizing expression vectors for for Protein Trans Splicing (PTS): pJJDuet30, pSFBAD09; and Native Chemical Ligation (NCL): pTWIN1 and pTWIN2. These vectors are modified to be compatible and more generally useful for other expression vectors that we use in the lab. Modifications include the insertion of a TEV cleavage site, as well as Trx and Z-fusion tags (Figure 26).

Initial expression and ligation tests using these vectors look very promising (Figure 27). Parameters that we are considering for optimization are:

- E.coli strains ER2566, BL21(DE3), BL21Star, Oligami, etc
- Temperature
- Induction timing
- Order of induction

We are currently doing molecular biology work with our model systems for expression tests with these vectors.

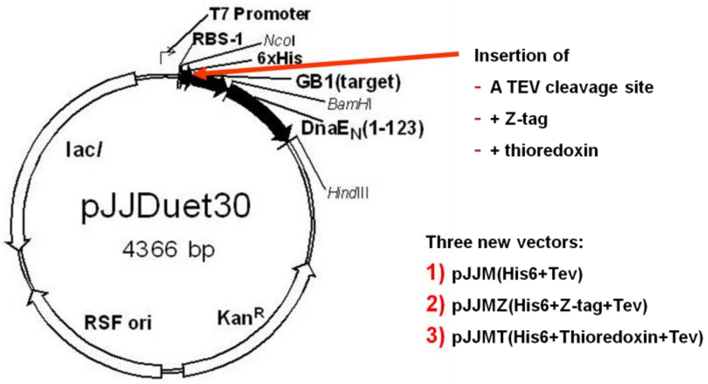


Figure 26: Modified expression vectors for protein trans splicing *in vivo.* The six-histidine tag and Z or thioredoxin fusion tag was inserted into the N-terminus of the fusion protein.

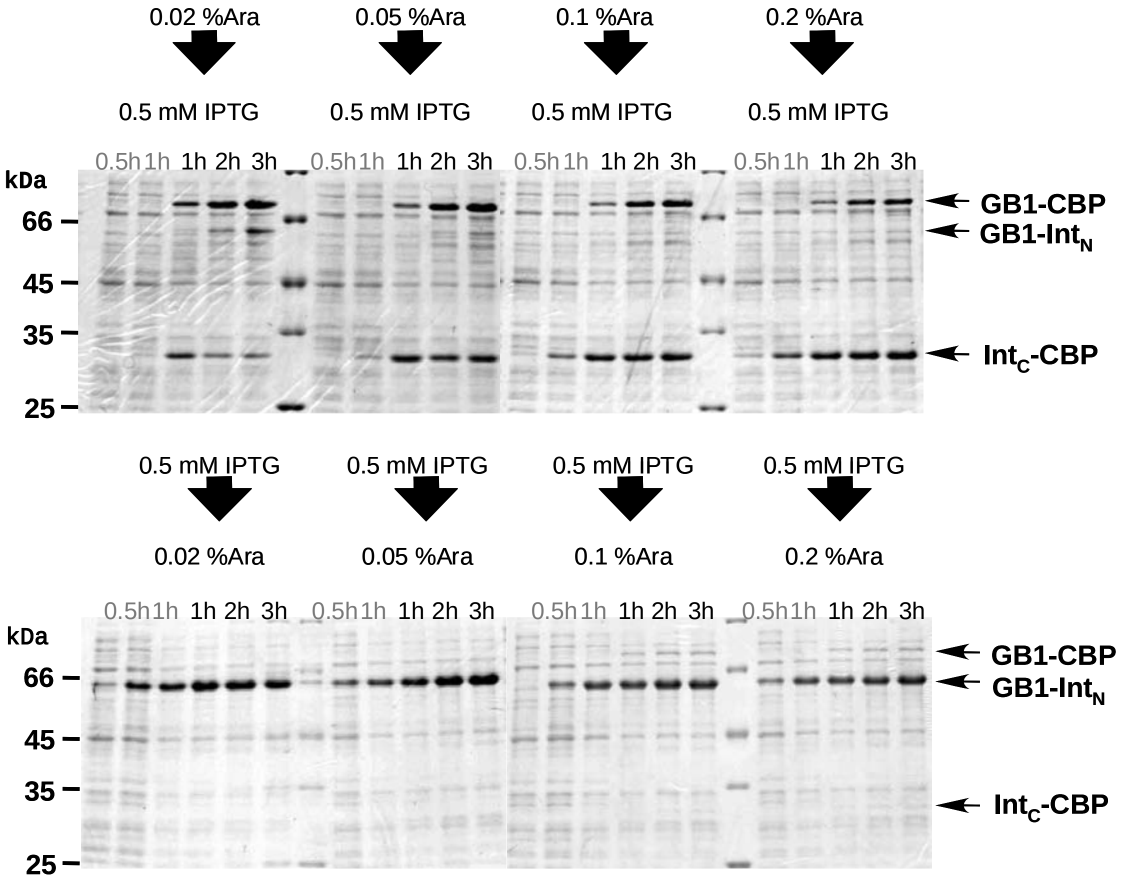


Figure 27: Expression and ligation tests using the pJJDuet30 and pSFBAD09 vectors for the N- and C-terminal fragments, respectively. GB1 was fused with N-terminus of the Intein on the N-terminal precursor expression vector, pJJDuet30, resulting in the fusion protein, GB1-Int$_N$. The Chitin binding protein (CBP) fragment was fused with the N-terminus of the Intein on the C-terminal precusor expression vector, pSFBAD09, resulting in the expressed fusion protein, Int$_C$-CBP. Depending on the order of induction using arabinose and lac promoter at varying concentrations and induction time quite different ligation efficiencies are obtained for the ligated GB1-CBP protein.

Publications/dissemination

Publications

Madl T, Felli IC, Bertini I and Sattler M
Structural analysis of protein interfaces from 13C direct-detected paramagnetic relaxation enhancements
(2010) J. Am. Chem. Soc. 132, 7285-7.

Madl T, Gabel F and Sattler M
NMR and Small Angle Scattering-based structural analysis of protein complexes in solution
J. Struct. Biol. *Submitted.*

Conferences/workshops

20.1.2010	ILL symposium "Molecules and membranes: the shape of things to come", ILL Grenoble, France
18.-23.4.2010	51st ENC, Daytona Beach, Florida, USA
17./18.5.2010	ESF-EMAR workshop on "Paramagnetic Tagging in NMR", Sevilla, Spain

Task 18.5: Low cost D-Glycerol production

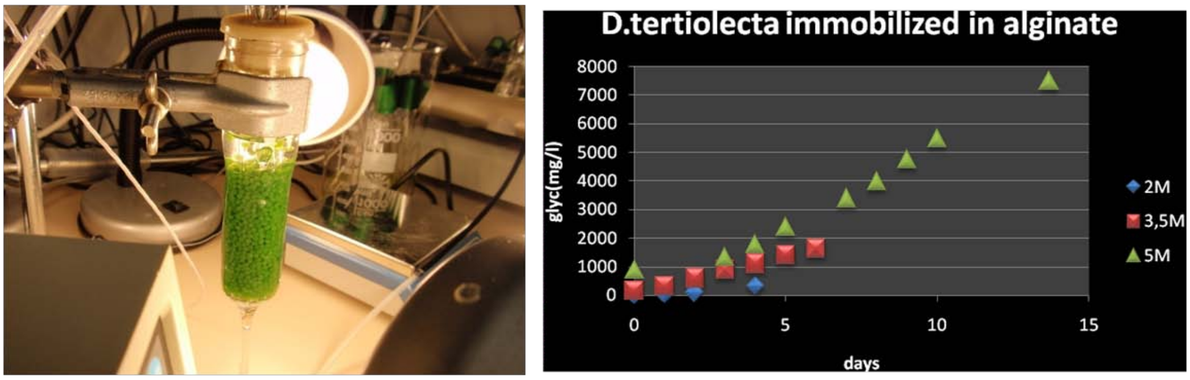
The high cost of deuterated carbon sources for the expression of D-proteins in E.coli or yeast is still a stumbling block for the application of neutrons in biology. The task is to develop a protocol for the production of D-glycerol. This approach is based on a milking process of algae, allowing repetitive use of the algae biomass thus substantially reducing the cost for the preparation of D-protein.
There are two mechanism of glycerol production by algae. Several algae strains e.g. those of the genus Dunaliella or Chlamodymonas produce glycerol as response to osmotic stress induced by salt. In previous studies we have used both strains for glycerol production.

Dunaliella:
Previous studies have shown that the salt tolerant algae strains of the genus Dunaliella can produce upon salt stress. Cells are grown in a medium containing 2M salt and subsequently transfered in a medium containing 5-6 M salt. As a response to the osmotic stress glycerol is accumulated intracellularly up to a concentration of 6M. The glycerol can be extracted after carefully collecting the cells without breaking. Collecting the cells by centrifugation allows toget rid of most of the salt. But exposure of the cells to salt concentration of 5-6M damages the cells irreversibly.
This procedure allows to produce glycerol, however, a cyclic milking process as previously anticipated, cannot be applied due to irreversible damage of the cells during the high salt exposure.

Chlamodymonas:
This sweet water strain can also be used for glycerol production. By applying a slight salt stress (100-200mM NaCl) facilitates continuous glycerol production. However the obtained glycerol concentration of 0.6 gr/ltr is too low for economic use.

Due to the low productivity of Chlamdymonas, we focused on Dunaliella as cell factory for continuous glycerol production.

Based on a published procedure, a milking procedure for glycerol production was developed. Cells are embedded in alginate and exposed to high salt conditions as described in Figure 28.



Algae cells were grown under low salt conditions (growth regime), embedded into alginate and transfered into a photoreactor (above left). Exposition of the cells to high salt (2M-5M NaCl) induced a time dependent excretion of glycerol (production regime). The highest amount was 7g/ltr (above right). The process can be improved by prolonging the milking time and by repetitive use of the cell biomass, indicating that the process is feasible for glycerol production (data not shown).

Figure 28: Photoreaktor using cells embedded into alginate

In the context of the recovery studies of cells after salt stress, we observed that cell growth and glycerol excretion depends strongly on the salt conditions; glycerol production can be performed continuously, if the strain is adapted to higher salt concentration.

Fig. 2 shows the results of an experiment in which the salt concentration was continuously increased until cell growth was inhibited (adaptation experiment). Conditions for continuous glycerol production were developed by an adaptation process, as shown in Figure 29.

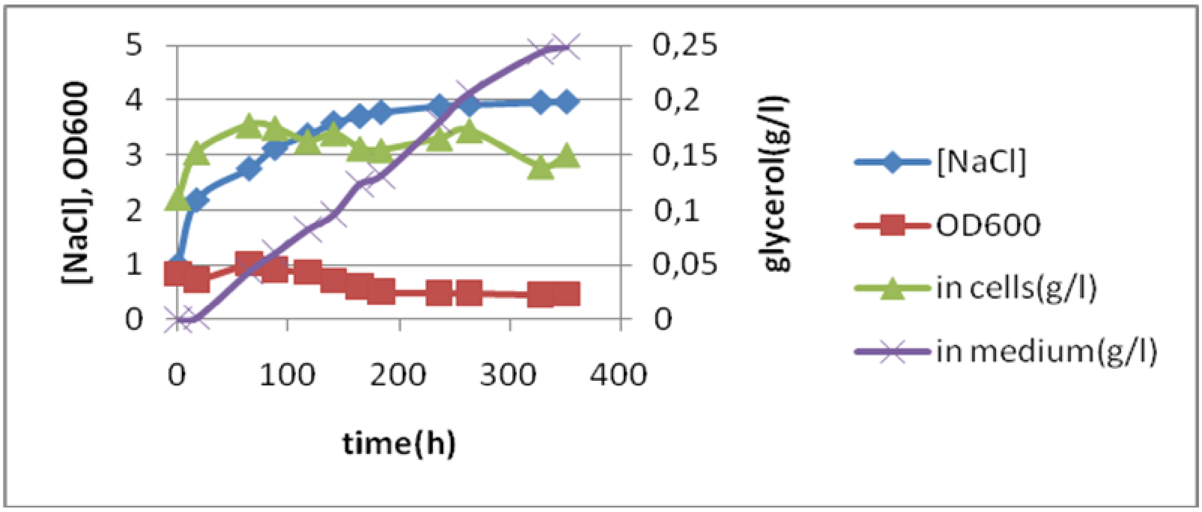


Figure 29: Continuous production of glycerol

The data show that glycerol is accumulated to 0,25gr/ltr. The cell division is reduced with increasing salt and glycerol concentration and fully inhibited above 2.8 M salt. The optical density slightly decreases, while the dry weight (g/ltr) doesn’t change after about 100h indicating that the size of the cells is decreasing with increasing salt concentration. Whether this is a time dependent effect due to exhaustion of the cell by producing glycerol or a salt dependent effect remains to be shown.

Figure 30 shows an analysis of the effectiveness of the glycerol production by determining the amount of C (delivered to the system by the carbon source, CO^2) in the intracellular, extracellular compartments and in the biomass. Fig. 3 shows that after 350 h 0,13 gr is in the intracellular compartment, 0,23gr in the media and approximately 0,075 gr in the biomass from a total amount of 1,25gr carbon from C02. It is not yet clear why the total balancing is not yet correct.

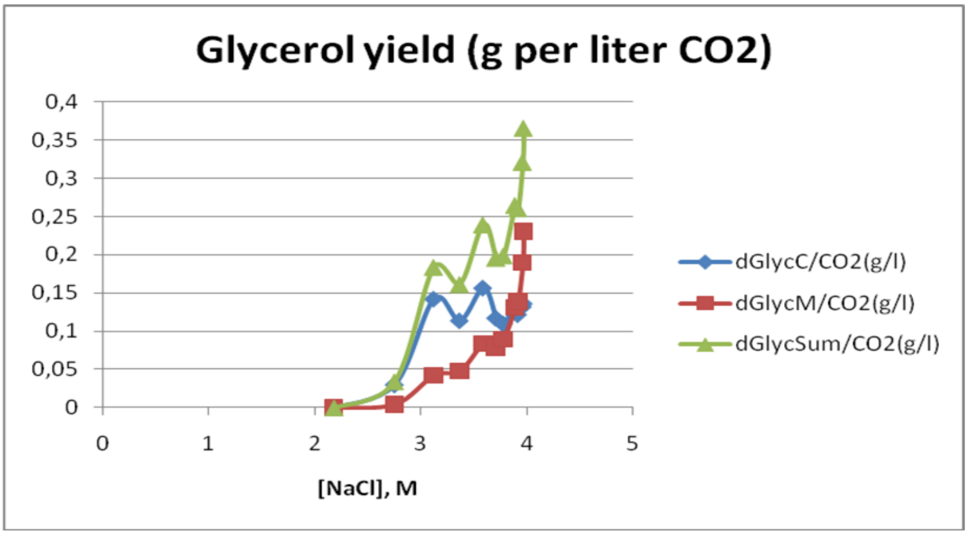


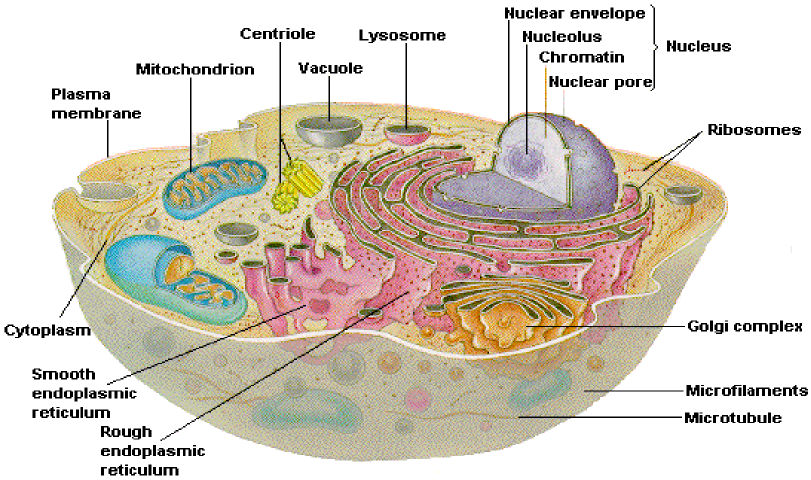
Figure 30: At 4M NaCl the overall glycerol yield reached a concentration of 0.36 g/l (0.23 g/l intracellular and 0.13 g/l extracellular), which means that approx. 26% of carbon was transferred from Co2 into Glycerol, indicating that the process is very effective

D-labelling:

Preliminary studies of the growth of Dunaliella in D2O indicated that the growth of this strain is greatly reduced in D2O above 95%. Further studies will be performed to solve this problem because the production of D-glycerol makes sense only if we can achieve enrichment above 98%.

Task 18.6: Deuterated membrane proteins

Membrane proteins perform a wide range of essential cellular functions and play key role in (for example) 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 sub task is focused on the development of methods to optimise deuteration of membrane proteins and their complexation with given surfactants for structural studies by SANS.



Model membrane proteins (OmpX, AcrB).

We selected: OmpX, expressed as inclusion bodies, is a small (16kDa) β-barrel monomer protein of the outer membrane; AcrB, expressed in the membrane, is a rather large (147 kDa) α-helical protein of the inner membrane. Purification protocols of the two proteins in their hydrogenated forms were checked. The report of our protocol for over-expressing OmpX in D_2O is free available[9].

Crystallisation of deuterated OmpX.

Manual screening was attempted in a variety of conditions which were successful for the hydrogenated protein. Three crystals were obtained without particular optimisation, e.g. in 0.1M citric acid pH 4, 20% v/v 2-Methyl, 2, 4-pentanediol. Their characterisation and optimisation is under way.

Production of deuterated FhuA (d-FhuA) (collaboration C. Breyton IBS Grenoble)

FhuA is the receptor of Phage T5 on the E. coli outer membrane. Expression of d-FhuA was done at the laboratory, using *E.coli* AW740 *[ΔompF zcb:TN10 ΔompC fhuA31],* a strain lacking the main porins of the outer membrane : OmpC and OmpF. The strain was transformed with the plasmid pHX405 containing the gene coding *fhuA* with an insert of 6 His in the loop L5, and an ampicillin resistance gene[10]. The strain was first adapted in a

[9] the detailed protocol "Lethier M., Moulin M., Härtlein M., Ebel C. Report on expression and purification of a deuterated model membrane protein: OmpX" is available on the web site of IBS: http://www.ibs.fr. Then search: SSIMPAS.

[10] A. D.Ferguson, J. Breed, K. Diederichs, W. Welte and J. W. Coulton, Protein Sci **7** (1998) 1636-8. An internal affinity-tag for purification and crystallization of the siderophore receptor FhuA, integral outer membrane protein from Escherichia coli K-12.

hydrogenated minimum medium before adaptation in a 80% deuterated minimum medium (described in http://www.ill.eu/sites/deuteration/index.htm). The adapted strain was inoculated to 3L of 80 % deuterated medium and the culture was grown at 37°C until OD_{600nm}= 3. 20g of cells were harvested. d-FhuA expression was successful as probed on Western Blot (Figure 32). The deuterated protein was purified according to [2] with minor modifications[11]. 6.6 mg of d-FhuA were obtained. Purity and deuteration level are attested by mass spectroscopy analysis (Figure 32)

Figure 32: Analysis by Western Blot of d-FhuA expression
1, 2, 3: 10µL of resuspended cells for each 3L of 80 % deuterated cultures + 5µLloading buffer.

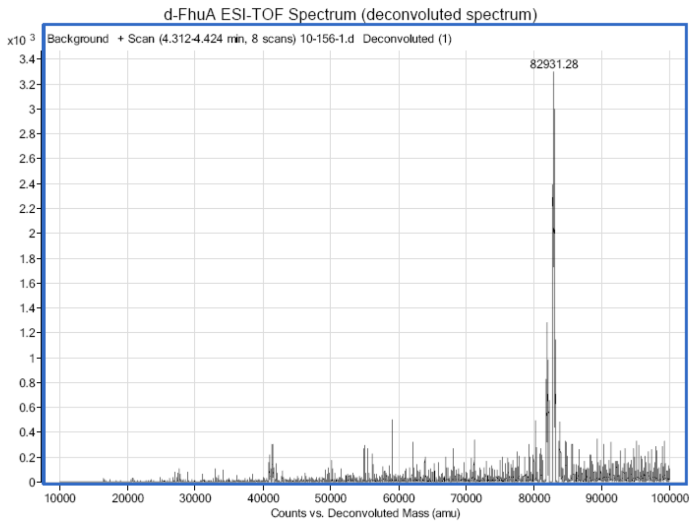


Figure 31: Analysis of purified d-FhuA by mass spectroscopy.

Detergent exchange for SANS studies

We initiated the study of the exchange for new fluorinated surfactants developed by B. Pucci (University of Avignon) and of interest for SANS studies[12]. We are evaluating different protocols (use of Biobeads, using affinity chromatography). We performed SANS studies on the new molecule F6DiGluM, and the comparison with deuterated detergents confirmed its potential interest (see below).

SANS experiments on d-FhuA solubilized by fluorinated surfactants

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[11] L. Plancon, C. Janmot, M. le Maire, M. Desmadril, M. Bonhivers, L. Letellier and P. Boulanger, J. Mol. Biol. **318** (2002) 557-69. Characterization of a high-affinity complex between the bacterial outer membrane protein FhuA and the phage T5 protein pb5.

[12] C. Breyton, F. Gabel, M. Abla, Y. Pierre, F. Lebaupain, G. Durand, J. L. Popot, C. Ebel and B. Pucci, Biophys J **97** (2009) 1077-86. Micellar and biochemical properties of (hemi)fluorinated surfactants are controlled by the size of the polar head.

After d-FhuA purification, the detergent was exchanged, using Ni-NTA affinity chromatography, to a fluorinated surfactant (F6diGluM, collaboration with B. Pucci Avignon) prior to SANS experiments on the instrument D22 of the ILL. Figure 33 and Figure 34 show the SANS scattering intensity measured at the matching point of the surfactant (46% D_2O). The results are extremely promising. Because the signal of the surfactant micelles is extremely low on a large Q-range, and the protein does not show any tendency to heterogeneity, the shape factor is expected to be evaluated with precision.

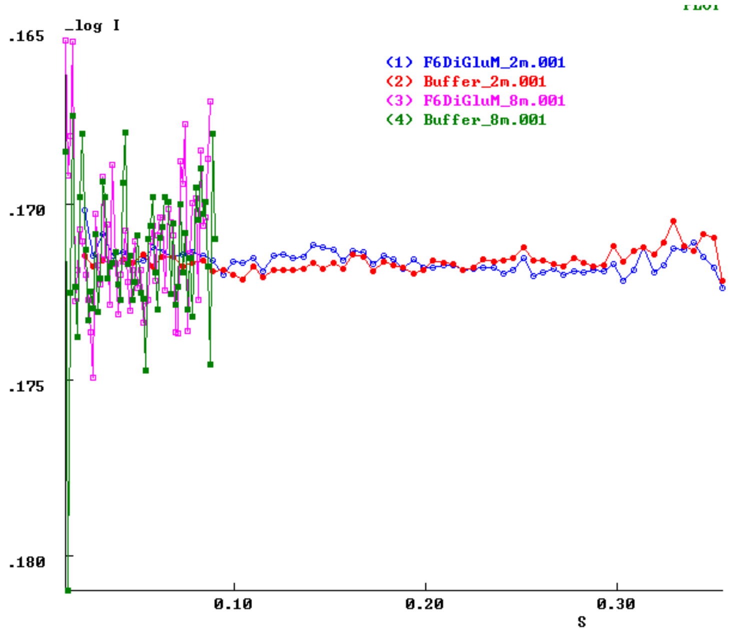


Figure 33: Superposition of the normalized by 1mm water signal scattered intensities obtained at two sample detector distances for F6DiGluM at 17.8 mg/mL and solvent ("Buffer"). Solvent is Tris-HCl 20 mM NaCl 0.15M, pH8, 46% D_2O.

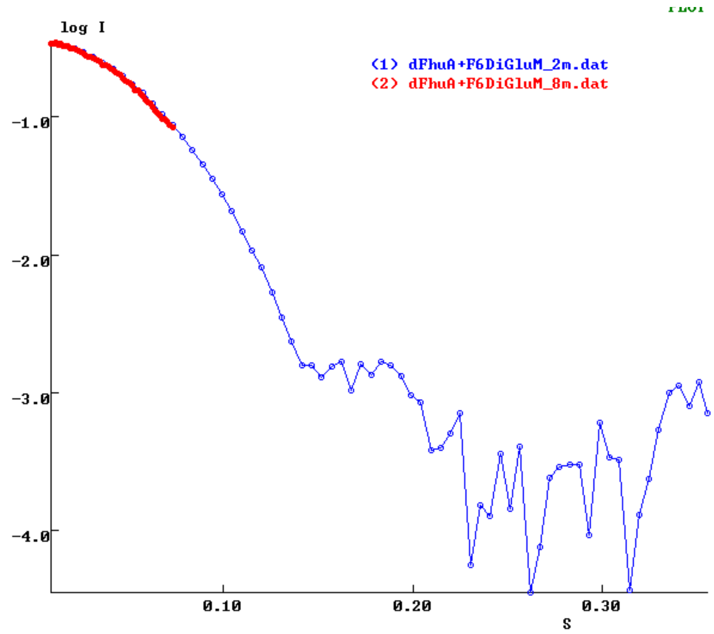


Figure 34: Superposition of the scattered intensities of d-FhuA at 4.3 mg/mL solubilized in F6DiGluM in the same solvent and the same experimental conditions as in Figure 3. Data are normalized by 1mm water signal and the signal of the solvent is subtracted.

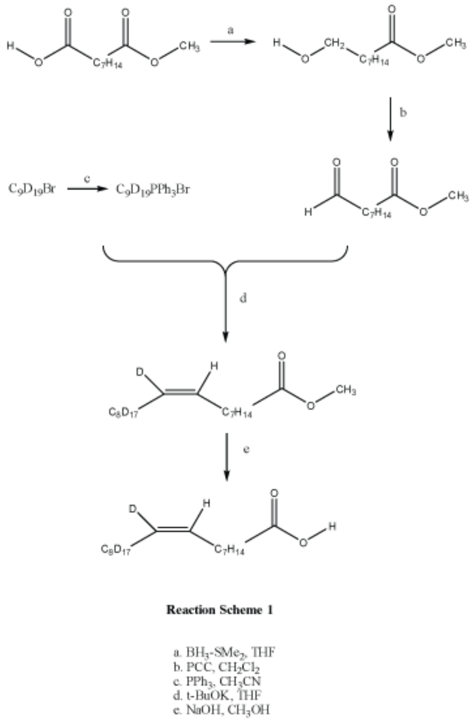
Task 18.7: Deuterated lipids

A growing range of biophysical and biochemical experiments on model lipid systems are being carried out using neutron scattering. These studies have been somewhat limited by the access to lipids of interest in deuterated form. In particular the limited access to unsaturated lipids has reduced the scope for carrying out both fundamental biophysical studies of the behaviour of unsaturated lipids in pure and mixed systems as well as more biologically oriented experiments on the structure and function of membrane systems where pure or mixed lipids system containing unsaturated components are known to be optimal.

We have identified through user consultation that access to lipids such as POPC, DOPC, POPG, and DOPG is desirable for preparing neutron experiments that more fully complement other biophysical techniques. Other, more exotic lipids are requested from time to time, but the challenges of preparing such molecules synthetically rule them out for the current project. Relatively few requests are made of mixed deuterated lipid systems of biological origin. This is likely due to the fact that most neutron users have a more strongly physical or biophysical perspective and therefore prefer to work with defined systems. We would expect, given the recent and expected future increase in use of neutron scattering by a wider range of biological scientists that the desire for such mixed systems in deuterated form will increase.

The first target of the task was therefore to identify an effective route towards deuterated lipids containing oleic acid, the ultimate target being delivery of useful quantities of this material. Broadly two synthetic routes to deuterated oleic acid from deuterated starting materials are possible, both involving the combination of a C9 deuterated chain precursor. Bromononane can be reacted with methyl 9-oxononanoate (see attached reaction schemes) or nonal can be reacted with methyl 9-bromononaoate. Both the methyl 9-oxononanoate and the methyl 9-bromononaoate are difficult and expensive to prepare in deuterated form. For both compounds the preparation of the intermediate monoester is an inefficient step. However, for the methyl 9-bromononaoate there is a further inefficient step where the COOH group is replaced by Br in the Hunsdiecker reaction. Furthermore, since the bromide must be used in 50% excess in the final Wittig reaction, there is additional wastage of the methyl 9-bromononaoate. We have therefore switched to the first route. The reaction schemes for the partially and fully deuterated oleic acids are shown as Scheme 1 and Scheme 2 below. This synthesis is currently being scaled up and multigram quantities are expected to be available soon.

The conversion of fatty acids to lipids is straightforward by established routes. We have elected to collaborate with a commercial supplier to carry out this synthesis as we believe this will provide the most efficient conversion and will enable rapid access to the final desired compounds. The collaboration will also help to assure the longer-term availability of these compounds to the neutron and wider research community by demonstrating a commercially viable demand for their synthesis. We note that the route above will also provide access to partially tail deuterated lipids (Figure 35) that may be of interest for spectroscopic and structural studies on the dynamics or position of different parts of the unsaturated lipid tail. We do not currently intend to prioritise production of these partially labelled molecules but will approach relevant groups to investigate the interest in such compounds over the next six months. Partially deuterated oleic acid can be made available for further conversion on a case by case basis. We expect to move to lipid production over the next six months and to be in a position to deliver gram quantities of the four proposed lipids by the middle of 2011.



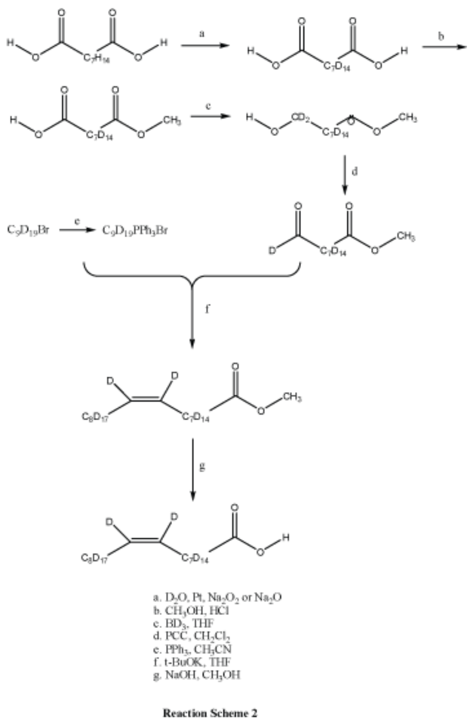


Figure 35: Synthesis of partially deuterated oleic acid. Scheme 2: Synthesis of perdeuterated oleic acid

Achievements

Task	Description / major progress	Partner
T18.2	Deuterated biomass	ILL
	D18.2.1.1 Report on identification of biomass system	ILL
	Algal systems (notably *Chlorella sorokiniana*) suitable for the production of perdeuterated biomass have been identified and conditions tested in hydrogenated media that will allow final protocols for perdeuterated biosynthesis to be optimised. The protocols involve novel photobioreactor technology. This task is of general interest for SANS, crystallographic and fiber diffrcaction work with neutrons.	
T18.3	Labelling of Pichia Pastoris	ILL
	D18.3.1.1Report of identification of expression systems	ILL
	Model yeast expression systems are being developed that are aimed at establishing optimised procedures for the production of a range of deuterated proteins that are not accessible using bacterial expression systems. *Pichia pastoris* is being used for this and the two model systems selected are human serine albumin (HSA) and lysozyme - both proteins of general interest for a wide range of biophysical studies using neutron scattering.	
T18.4	Segmental labelling	TUM
	D18.4.1.1 report on model system designs	TUM
	There is a huge requirement (in SANS, reflection, and fibre studies using neutrons) for proteins where extended regions/domains/subunits are selectively deuterated. Protein splicing approaches for this type of segmental deuterium labelling are being developed.	
T18.5	Low cost D-glycerol production	MPG
	D18.5.2.1 Report about the milking process, small amounts of glycerol	MPG

	In this task, methods are being developed for the production of deuterated glycerol by algae under salinic stress. The idea is that the deuterated glycerol thus produced is then available for use in feeding bacteria, with the ultimate goal of reducing the effective cost of this compound, thereby widening access by reducing the cost of deuterated biomolecules for neutron scattering studies.	
T18.6	Deuterated membrane proteins	CEA (IBS)
	D18.6.1.1 report on the optimised production of a model protein	CEA (IBS)
	Membrane proteins perform a wide range of essential cellular functions and play key role in (for example) transportation, energy management, signal transduction, photosynthesis. Neutron scattering studies using appropriately labelled samples provide powerful insights to these systems. This task will is focused on the development of methods to optimise deuteration of membrane proteins.	
T18.7	Deuterated lipids	STFC
	D18.7.1.1 Report on targets and proposed routes	STFC
	A growing range of biophysical and biochemical experiments on model lipid systems are being carried out using neutron scattering. These studies have been somewhat limited by the access to lipids (in particular unsaturated lipids) of interest in deuterated form. This task is focused on the production of partially deuterated oleic acid and the subsequent move to lipid production over the next six months.	

WP19 POLARIZED NEUTRONS

Objectives

1. Develop and make available the wide-angle polarization analysis for neutron diffraction/spectroscopy

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

2. To extend possibilities of methods of Larmor labelling towards higher energy and momentum resolution.

The Larmor labelling of individual neutrons allows the development of “unusual” neutron scattering techniques. An extremely high energy (momentum) resolution that is not possible in conventional neutron spectroscopy (diffraction) because of intolerable intensity losses, become achievable. The Larmor labelling also opens exciting possibilities for further developments of polarized neutron techniques, such as measurements of three/many point correlation functions, the generation of pulsed beams out of continuous polychromatic beams, etc. research.

3. To broad the user base of polarized neutron scattering by an extensive education and training program.

We will continue the proven to be successful practice of the organization schools on polarized neutron scattering.

Work progress

Task 19.2: Development of wide-angle polarization analysis in neutron diffraction and spectroscopy

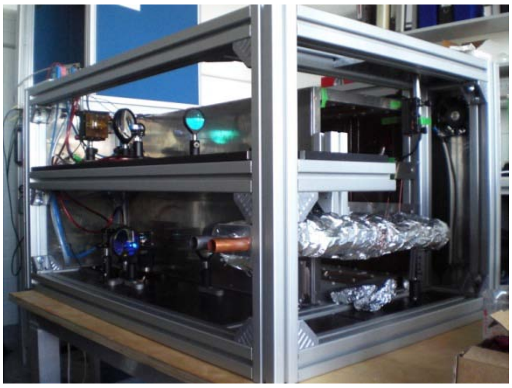
Sub-task 19.2.1: Large solid angle polarization analyzers

The largest in the world 3He cell made of the GE180 glass (Figure 36) was manufactured in the FZJ aiming to be installed in the front of large PSD detector at the reflectometer MARIA at JCNS. The setup for the on-beam pumping using two diode bars was designed, constructed and tested. The on-beam polarization 80.2% was achieved and maintained constant within 2 days.

To discuss the current state of the art in the filed the workshop on "Wide Angle Polarization Analysis in Neutron Scattering" (WAPANS) was organized by the JRA and held in Paris on 22.2.2010. It was attended by JRA partners and observers, scientists from Australia and USA as well as representatives of commercial firms –producers of super mirror polarizers. It was reported about a number of wide-angle supermirror analyzers that have been developed and manufactured.

Based upon the results of these discussions, the decision about the design of analyzers for the diffractometer Super 6T2 at LLB and spectrometer TOPAS at JCNS will be taken to the end of 2010.

Figure 36: The largest in the world 3He cell made of the GE180 glass manufactured in the FZJ.



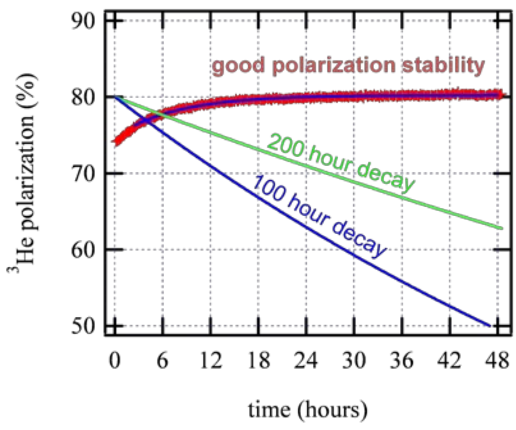


Figure 37: Picture of in-situ SEOP polarizer and the time-dependence of the 3He polarization for the on-beam pumping (red) compared with T1=100h (blue) and T1=200h (green).

Sub-task 19.2.2: Large solid angle magnetic environment friendly spin-handling devices

A new magnetostatic cavity allowing to achieve the magnetic life time of 3He up to 1000h in very large cells was developed. The dedicated software allowing for quick simulations of different magnetic scenarios for 3He cells is installed and under the test. It will become available to all partners within 2 months.

Task 3. Further developments of Larmor labelling methods for inelastic neutron spectroscopy

Sub-task 19.3.1: Correction elements for high energy resolution

Twelve crossed Pythargoras coils (Figure 38) with thickness modulation and straight cuts each with an active area of 100x100 have been produced and are build in the J-NSE spectrometer in Garching (4) and the SNS NSE spectrometer (6). They already improved the performance of J-NSE significantly. The SNS-NSE setting is currently being put into operation.

The 100x100 mm^2 active area is sufficient for the incoming beam correction and for the correction elements close to the sample in the secondary arm. However, in order to better utilize the 300x300mm^2 a larger area of the last correction coil is needed. As a step in this direction two 160x160mm^2 sets of Pythargoras coil sets have been produced featuring also inclined cuts to smoothen the projected current distribution function. Since the coils are located at some distance from the detector the covered detection area is about 220x220mm^2. In addition to the parabolic correction of these coils for the large diameter an additional weak corrector for the higher order polynomial coefficients is needed an to be tested with neutrons. The making of first approaches to these items in the form of copper on capton spirals is currently under progress.

In order to limit the temperature developed by the Pythargoras coils that perform the main part of the corrections, the central mounting plates have been remade with water cooling channels. A test of the efficiency of this measure has been performed with the large correctors. (Figure 39)

Upcoming are now neutron tests (first at the J-NSE and then at SNS) of the completed set of Pythargoras coils and the need and efficiency for/of the higher order correction for the larger area.

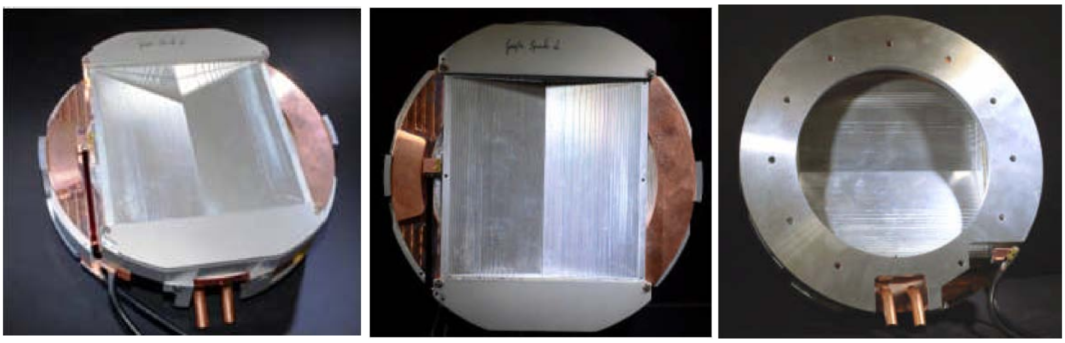


Figure 38: Assembly of a new large set of Pythargoras coils with central water cooling.

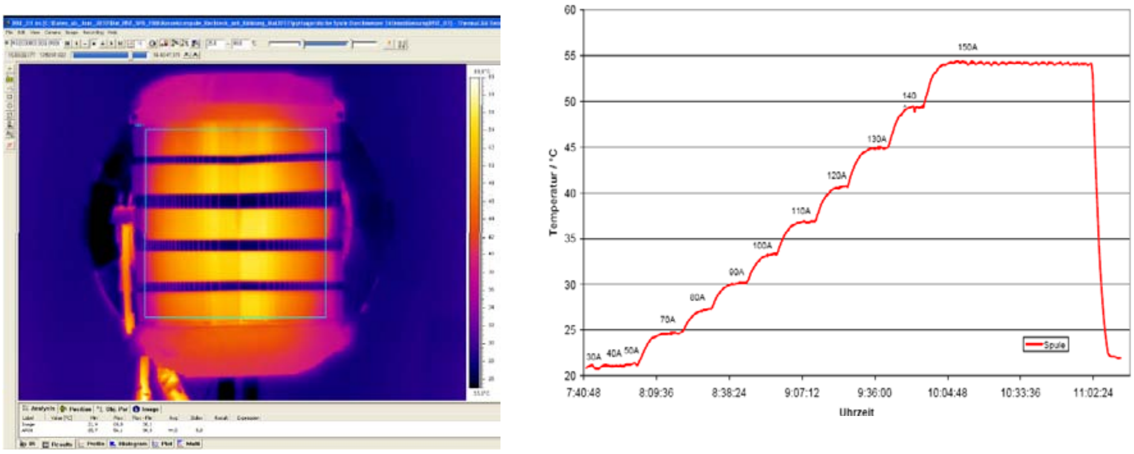


Figure 39: Maximum temperature of coil surface as function of current and time, with water cooling on, as derived from the thermographic image (left)

Sub-task 19.3.2: Development of a large-(Q,ω)-range inelastic neutron scattering spectrometer based on a combination of time-of-flight and Larmor labelling (TOFLAR)

A start has been made of the theoretical description and analytical modelling of the TOFLAR technique. The measured intensity as a function of ToF and the magnetic field *B* of the Larmor modulator is expressed in terms of the dynamic structure factor.

The instrument is simulated by Monte Carlo. For this purpose further developments of the simulation package McStas have been undertaken. Tools for polarization in the McStas kernel and components for polarized neutron control, precession, scattering, and monitoring have been set up. Particularly, a description of neutron polarization has been added to the kernel, as well as support for external time-constant magnetic fields, spin precession, polarizing optics (perfect polarizer, polarizing mirror, polarizing guide, Mezei spin flipper), polarization monitors, polarization visualization, polarizing samples. A start is made to compare the analytical and simulated results.

A prototype has been built at RID, Delft (Figure 40) and first test measurements on water and acetone samples were performed. Results are given in Figure 41. The extra damping of the signal compared to the modulation in the straight beam is a result of the inelastic scattering from the sample. Results have been presented at the PNCMI conference.

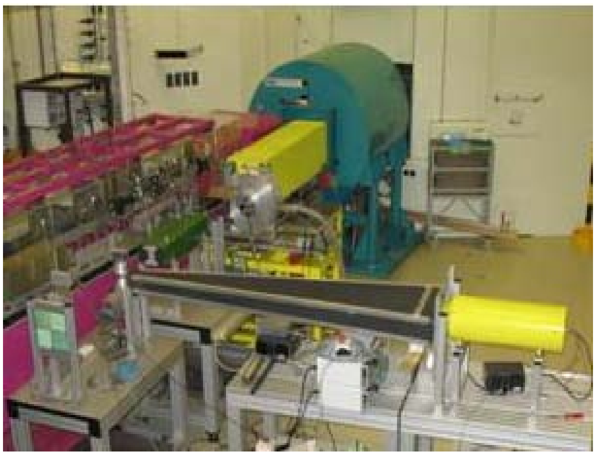


Figure 40: Prototype TOFLAR setup at RID, Delft

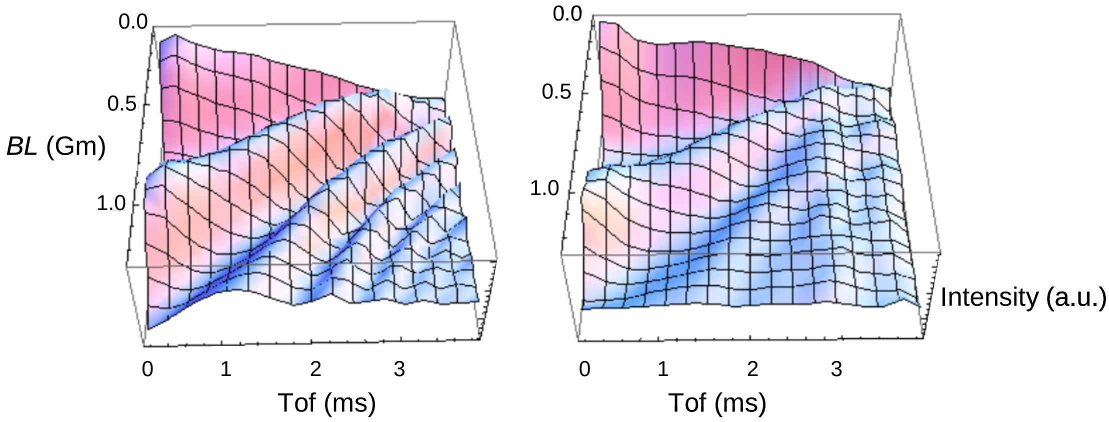


Figure 41: Measured intensity as a function of time of flight and magnetic field in the Larmor modulator for the straight beam (left) and the scattered beam from a 2-mm-thick acetone sample at a 90° scattering angle (right).

References: M. Bleuel, A.A. van Well, *First tests of the new TOFLAR (time of flight and Larmor precession) method*, (PNCMI2010) Physica B, submitted

Task 4. Further developments of Larmor labelling methods for SANS and reflectometry.

Sub-task 19.4.1: Larmor labelling with rotating magnetic fields and time-gradient magnetic fields

A new neutron-spin echo technique based upon the use of time-gradient magnetic fields, TGF NSE, can be used for purposes of small-angle neutron scattering and reflectometry. It employs simple solenoids as spin turners, thus allowing for a construction of long coils that can be tilted to rather small incident angles as it is requested for high-resolution angular measurements. However, in contrast to the use of static or radio-frequency magnetic fields as in the well-known SESANS, the use of time-gradient magnetic fields results in the unusual dependence of the spin-echo length from the neutron wavelength: λ^3 rather than λ^2. This allows for a significantly higher Q-resolution and for a very significant increase of Q-range with the latter feature especially valuable for the time-of-flight operation mode at pulsed neutron sources. Theoretical analysis of the TGF spin-echo small-angle neutron scattering /reflectometer setup has been carried out (Figure 42). Special components for the VITESS simulation package has been developed and tested. The simulation of the setup is in progress.

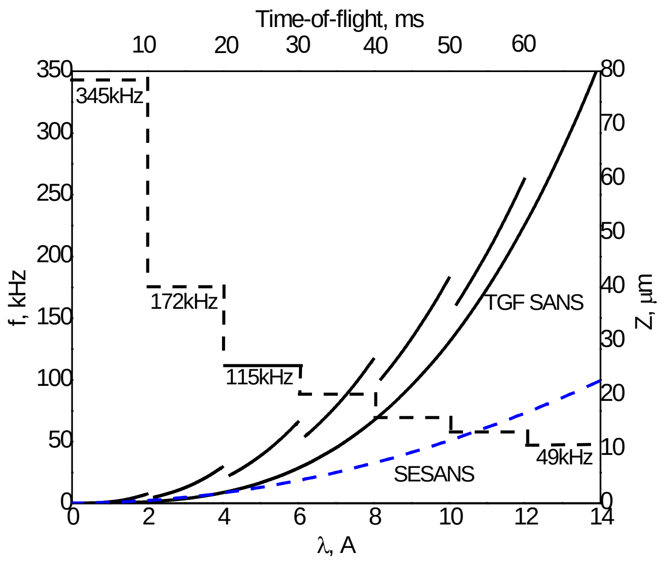


Figure 42: . Comparison of $Z_{TGF\ SANS}$ with $Z_{OFFSPEC}$ spin-echo times.

Sub-task 19.4.2: SANS and reflectometry with MIEZE

Several experiments using the MIEZE technique in combination with SANS measurements have been performed at instruments MIRA and RESEDA (2009). Using MnSi (a helimagnet) in the zero-field regime a good agreement with NRSE data from preceding RESEDA measurements was found above and below Tc of 28.5 K. These experiments proved that the MIEZE technique is working at both instruments and delivers valid results.

In 2010 additional experiments on MnSi were performed in a magnetic field at MIRA. Here the so-called A-Phase and the conical phase were studied in detail. For these experiments, the small angle picture from the MnSi was remeasured using a x,y-table for the MIEZE single detector. Thus, the intensity distribution could be measured and the detector could be positioned at the relevant positions. At these positions, MIEZE data were taken for different temperatures and magnetic fields. The data evaluation of these measurements is ongoing, but it could already be shown that such a combination of SANS and MIEZE measurements is feasible.

For future experiments, a new position- and time-resolving detector (the CASCADE detector from Heidelberg) was ordered for both instruments. These detectors are currently being manufactured and will considerable speed up the measurements.

Within the task 19.4, we performed several experiments using the MIEZE technique in combination with SANS measurements. Within the task 19.4, we performed several experiments using the MIEZE technique in combination with SANS measurements: on the instruments MIRA and RESEDA. MnSi - a helimagnet - was measured in the zero-field regime and good agreement with NRSE data from preceding RESEDA measurements was found above and below T_c of 28.5 K. These experiments proved that the MIEZE technique is working at both instruments and delivers valid results (Figure 43a).

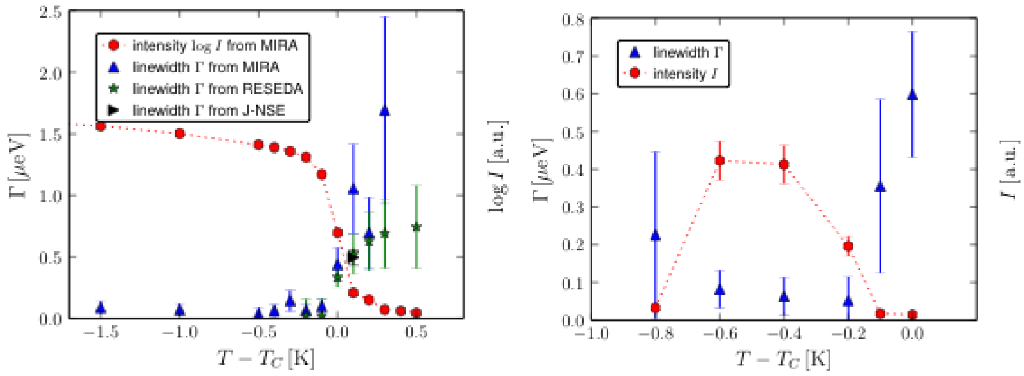


Figure 43: *(a)* *(b)*

Sub-task 19.4.3: Correction elements for high momentum resolution

A study has been made on spin flippers, where field flippers are distinguished in high and low field flippers. Low field flippers can been used in normal polarized neutron experiments, while high field flippers are required in SESANS and high resolution Larmor diffraction to achieve strong gradients in Larmor precession angles. Examples of the last ones are resonant flippers and magnetized foil flippers. Experimental and theoretical work was performed on flippers of magnetized Permalloy foils using a moving domain wall parallel to the foil surface in order to achieve the proper flipping conditions in a time of flight (ToF) beam for all wavelengths. From simulations of the system a clear insight was obtained in the experimental problems to be solved.

- The possibility was studied theoretically and experimentally of a vibrating foil that changes its beam transmission length, in such a way that all wavelengths in a ToF beam precess over 180 degrees.
- A study was made of the influence of geometric phase rotation in spin echo set-up for white beams. These phases occur using flippers of the adiabatic type, but it appears that the geometric effects can be avoided using certain symmetry conditions in the application.
- Finally an overview was written of the Larmor precession techniques in the last fifty years.

References:

1. Theo Rekveldt, *Larmor labeling Development*,(PNCMI2010) Physica B, submitted
2. Theo Rekveldt, Wicher Kraan, *Spin flippers for Larmor labeling methods in monochromatic and white neutron beams*, Nucl.Instr.&Methods in Phys.Res.A, submitted.
3. W.H.Kraan, S.V.Grigoriev, M.T.Rekveldt, Phys.Rev. A82,013619 (2010).
4. W.H.Kraan, S.V.Grigoriev, M.T.Rekveldt, *Observing the build-up geometric precession phase in an adiabatic RF flipper with the amplitude of its rotating field,* (PNCMI2010) Physica B, submitted

Task 5. Developments of wide-angle neutron resonance spin-echo

Sub-task 19.5.1: NRSE coils: high fields, new field geometries

This subtask focuses on the development of the large solid angle NRSE coil being used as the first NRSE coil after the sample position. This coil is supposed to allow for a detector solid angle of 30 degree. Therefore, the coil has to be relatively wide, compared to conventional NRSE coils (Figure 44)

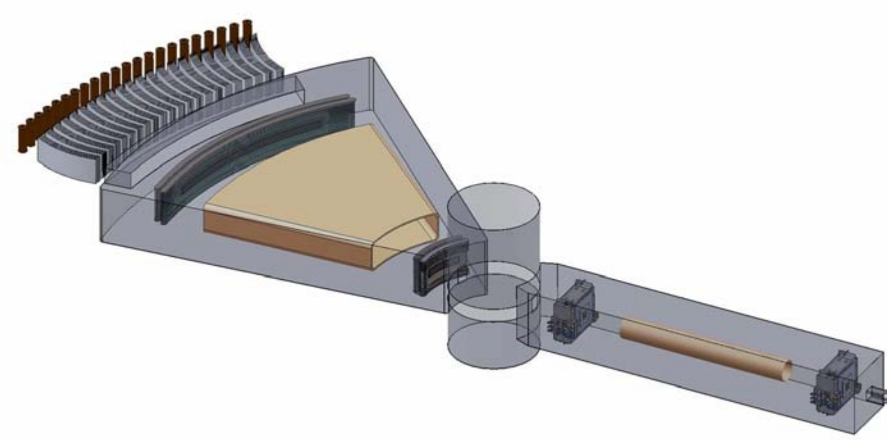


Figure 44: General design of the Multi-detector NRSE spectrometer

We started the design of the first curved coil which corresponds to the shorter radius of curvature and thus the most difficult to realize with a good field homogeneity (Figure 45). We also designed and constructed new flat coils that should be located in the first arm. New principles were developed in order to improve the field homogeneity (better resolution quality) and the maximum reachable frequency (maximum spin echo time).

A first exemplar of these coils has been tested in May (resonance part) and beginning of July (all coils) by the resonance spin-flip at the MUSES spectrometer of the LLB. The quality is more than satisfactory because currents as high as 100 A could be used for a long time with a maximum temperature of the coils (in the beam region) of 28°C. This cooling condition was absolutely mandatory for the curved coils since dilatation of the mechanical structure should be avoided. HF current stability and good quality spin flips were obtained. The test of the coil homogeneity over the beam region by the use of masks also gives satisfactory results. The construction of other flat coils is in progress.

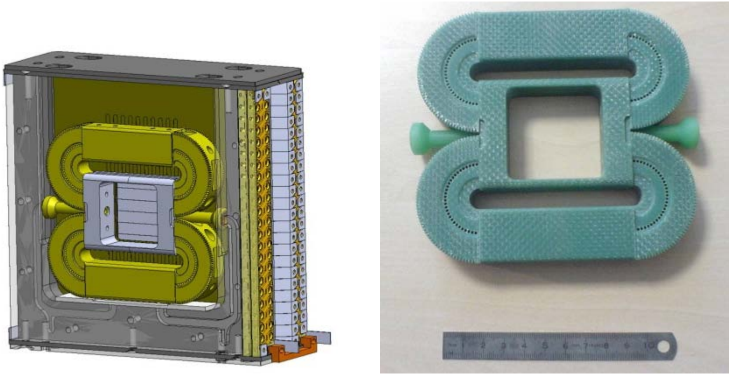


Figure 45: Design and construction of new type flat NRSE coils for the first arm has to be curved with respect to the sample position. Due to the curved shape, the large solid angle coil cannot be easily wound to a coil body, as NRSE coils are normally produced, but they rather have to be manufactured by means of alternative techniques.

In order to acquire the needed know-how concerning the manufacturing technique and the thermal and mechanical stability of such coils, in a first step, the manufacturing and cooling technique are developed and tested on standard-sized NRSE coils. Finishing in February 2010, we have constructed small cooling plates which can be scaled up to a large solid angle cooling plate. They consist of a body with channels for the cooling liquid, and a plate fitted water-tightly to the body. These parts will be used for the low solid angle NRSE coils which are needed in the first arm and in front of the detector of a large angle NRSE setup. In addition, they will be scaled up for the being used for the new large angle coil.

In addition, magnetic field simulations have been performed, in order to optimize the field homogeneity of large solid angle NRSE coils. In contrast to standard used bootstrap NRSE coils, where the magnetic flux is closed by a pair of NRSE coils placed next to each other, the large solid angle coil will be constructed with a mu-metal yoke closing the magnetic flux of one single coil. The magnetic field simulations show, that optimization of the geometry of such a yoke allows for the realization of a sufficiently homogeneous magnetic field.

In the next steps, the mechanical support for a large solid angle NRSE coil will be planned and constructed. After this, the construction details, including the electrical contacting technique will be discussed, also with the manufacturer.

Realization of wide-angle neutron resonance spin echo (NRSE) affords the development of new NRSE coils, which define the spin precession region of neutrons scattered into a large solid angle range. Task 19.5.1 focuses on the development of the large solid angle NRSE coil being used as the first NRSE coil after the sample position. This coil is supposed to allow for a detector solid angle of 30 degree. Therefore, the coil has to be relatively wide, compared to conventional NRSE coils, and it has to be curved with respect to the sample position. Due to the curved shape, the large solid angle coil cannot be easily wound to a coil body, as NRSE coils are normally produced, but they rather have to be manufactured by means of alternative techniques.

In order to acquire the needed know-how concerning the manufacturing technique and the thermal and mechanical stability of such coils, in a first step, the manufacturing and cooling technique are developed and tested on standard-sized NRSE coils. We have constructed small cooling plates which can be scaled up to a large solid angle cooling plate. They consist of a body with channels for the cooling liquid, and a plate fitted water-tightly to the body. These parts will be used for the low solid angle NRSE coils, which are needed in the first arm and in front of the detector of a large angle NRSE setup. In addition, they will be scaled up for the being used for the new large angle coil (Figure 46).

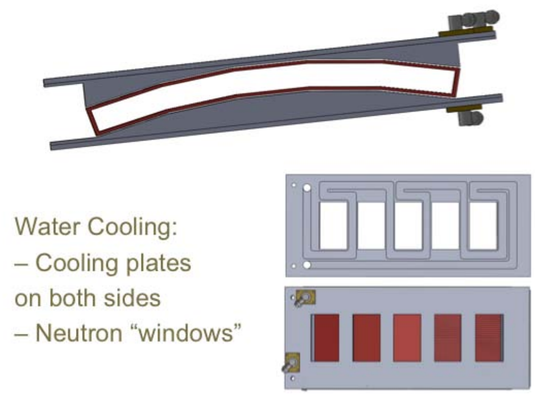


Figure 46: Cooling techniques on NRSE coils

Sub-task 19.5.2: NRSE coils with minimized amount of material in the beam

The curved resonance coils are the critical difficulty we have to overcome to realize the project. The coils are made of a vertical static of the order of few hundred Gauss in which are inserted a radiofrequency coils used in the frequency range between 50KHz and 1MHz. In order to produce an echo two coils are necessary per arm.

We started the design of the first curved coil which correspond to the shorter radius of curvature and thus the most difficult to realize with a good field homogeneity. We also designed and constructed new flat coils that should be located in the first arm. New principles were developed in order to improve the field homogeneity (better resolution quality) and the maximum reachable frequency (maximum spin echo time). These coils are going to be tested soon and if the quality is satisfactory we will start the construction of similar curved coils within the 6 next months.

Another approach is developed by the LLB partner, who designed a curved coil in the beginning of 2010 and the construction and test of the RF coils should be achieved before the end of the year. The mechanical part with cooling circuit and the static part of the coils are planned at the beginning of 2011 and the realization should be performed within the end of the year by the way it is shown on Figure 47.

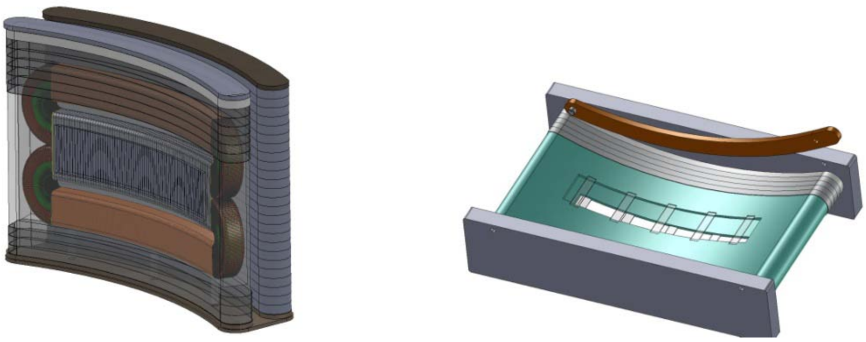
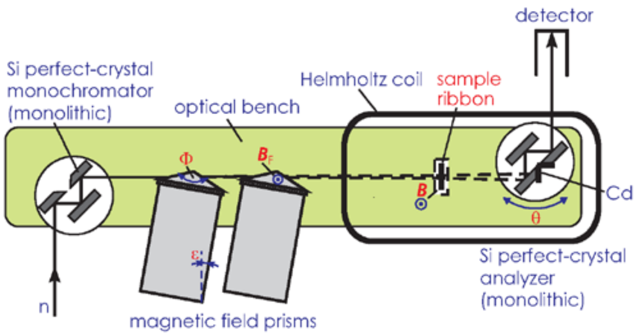
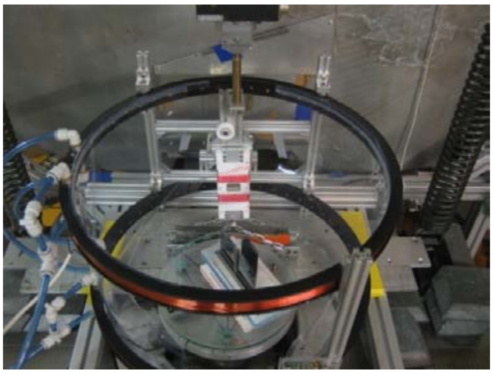


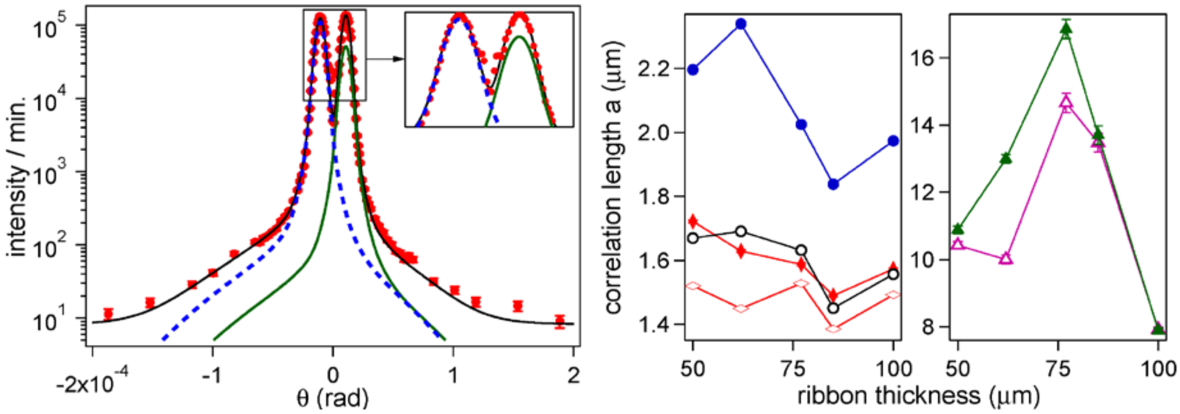
Figure 47: Design of the curved resonance coil of the second arm of the NRSE spectrometer

Task 6. Development of new polarized neutron techniques

The ILL CRG-B instrument S18 may now be used routinely for USANSPOL measurements. Sample environment for characterization of magnetic samples under external magnetic fields and applied mechanical stress was developed and is currently in prototype status. Continuous development towards user operation is foreseen. The instrument has been tested with various amorphous soft-magnetic ribbons with novel magnetostriction properties.







Software and modeling is being developed for data analysis. The lower part of the figure shows how models may be applied to separate spin-up and spin-down neutron scattering and to visualize the interference of magnetic and nuclear scattering. From these data average size parameters of the scatterers can be derived which may be used to investigate the evolution of magnetic structures under varying environmental conditions and to characterize samples which were produced under different manufacturing conditions. This is illustrated in the lower right corner of the figure for 5 different Galfenol ribbons studied under increasing external magnetic field.

The project is well underway, there are no deviations from the task's timetable.

USANSPOL layout (top left); analyzer part of the instrument with several magnetic coils to provide or cancel out external magnetic fields (top right); data analysis of polarized neutron scattering (bottom left) and sample characterization of Fe-Ga alloys using the USANSPOL technique (bottom right).

Sub-task 19.6.2: Development of an ultra-flexible neutron magnetic resonator

A PhD student has been hired and he started his contract in December 2009, the 12 man-months foreseen for TUW/ATI in this task will be completed by the end of November 2010. Additional funding for this project has been granted by Austrian national science funding (FWF project I 528-N20 "MONOPOL") which will enable the completion of the doctor thesis. With this funding the acquisition of power supplies which are essential to the project has become possible. Given this context, the project is well underway and there are no deviations from the task's timetable. A series of numerical simulations has been performed in order to investigate in detail the performance of specific spin resonator configurations and to find out the optimal design parameters prior to an actual experimental realization. At first the 3-dimensional magnetic field distribution of the respective resonator configuration was calculated by means of the commercially available simulation software CST-Studio Suite™, which was then used as input to VITESS, a virtual instrumentation tool for neutron scattering at pulsed and continuous sources. As a typical example, the resulting polarization behind a stack of 18 individual Al current sheets (20×10×0.03 cm^3) is shown, which were separated periodically by a distance of 1 cm. A resonance wavelength of 5 Å was chosen, corresponding to a homogeneous vertical field component B_0 = 1.357 mT. Full spin flip was achieved at an average resonator current of 18.15 A. 'Sinc'-shaped amplitude modulation of the oscillatory transversal field (B_1^{max} = 0.118 mT) was used to suppresses subsidiary maxima. The decrease of spinflip probability with increasing beam cross-section arises from field inhomogeneities at the current sheet boundaries. In the final design of a pulsed resonator, which will be operated in a ‘travelling’ wave mode to allow decoupling of wavelength and time resolution, these sheets will therefore be replaced by low-inductance coils made of Al ribbons, as indicated in the figure.

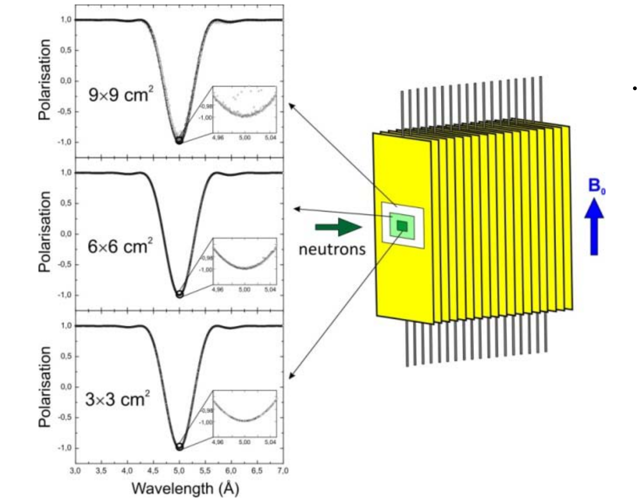


Figure 48: Numerical simulations of the polarization behind a resonator consisting of 18 separate current sheets separated by a distance of 1 cm for three different beam cross-sections. A ‘sinc’-shaped modulation of the oscillatory A ‘sinc’-shaped modulation of the oscillatory transversal field was used to suppress subsidiary maxima.

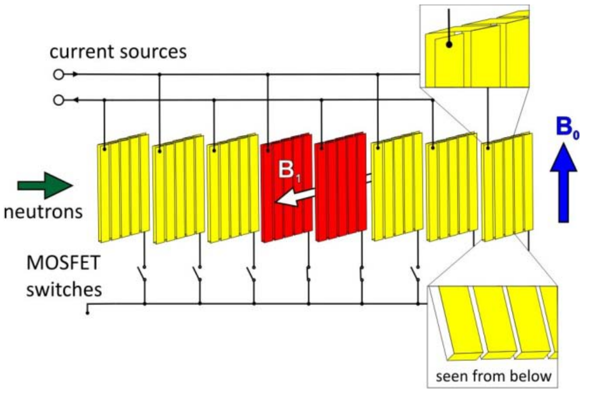


Figure 49: Low-inductance Al-ribbon coils will likely be the optimal choice for the final resonator design.

Sub-task 19.6.3: Polarized neutron technique for measurements of three/many point correlation functions

The prototype setup for the Four-Wave Neutron Resonance Spin Echo (FW-NRSE) experiments have been built at the beam N14 of the reactor WWR-M operating at 14 MW power at PNPI, in Gatchina, Russia. In such setup spin precession produced by a couple of the neutron resonance coils should be compensated by the identical couple of the other coils, thus performing as two arms of a spin echo machine.

The monochromatic beam at $\lambda = 0.23$ nm ($\Delta\lambda/\lambda = 0.02$) is polarized by the polarizing mirrors and analyzed by the similar mirror upstream of the detector. NSE arm 1 consists of two electromagnets with the field up to 4 kG acting in the ordinary mode without RF coils. NSE arm 2 consists of two electromagnets with RF coils acting in the resonant mode. The measurements were performed at different settings of the spin flip probabilities ρ of the RF flippers and different frequencies of the RF coils. Figure 1 demonstrates the SE pattern obtained at the RF frequency of the RF coils is 1 MHz and with the corresponding magnetic field equal to 36 mT. The pattern is obtained at $\rho = 0.42$.

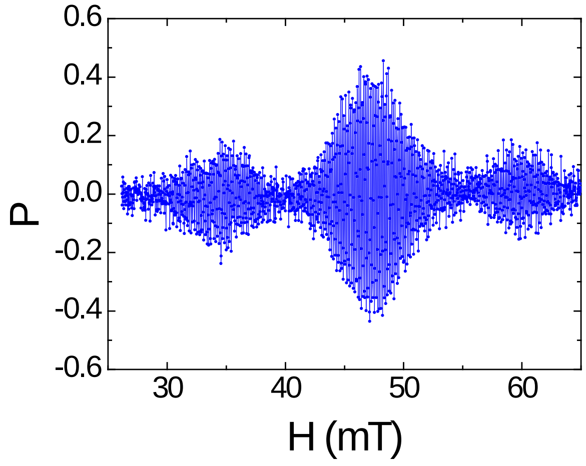


Figure 50: SE pattern as a function of the magnetic field H in the electromagnets of SE-arm 1 and at frequency f = 1 MHz at the spin flip probability ρ = 0.42 of the RF coils of SE-arm 2.

The frequency range to operate the setup is ranged between 0.2 and 2.4 MHz. The experiments were performed at different values of the frequencies and SF probability of the RF coils ρ = 1 and the amplitude of the SE patterns were measured. Figure 2 shows the amplitude of the SE pattern as a function of the RF frequency f taken at the spin flip probability ρ = 1 of the RF coils. The amplitude is rather low of order of 0.3- 0.5 because of the loss of the polarization along the path of the neutron beam. On the other hand, the amplitude does not change much upon increase of the frequency and therefore loss of the polarization is not related to the magnetic field and to the RF option but rather to the nonadiabatic passage close to the pi/2 rotators. The measures to gain the loss the polarization should be taken in the nearest future.

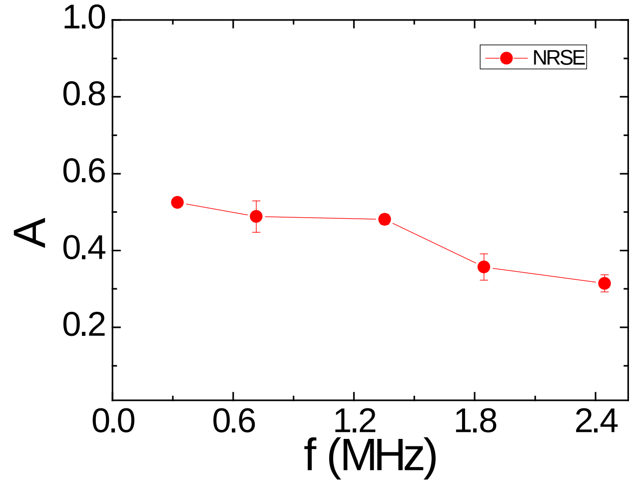


Figure 51: Amplitude of the SE pattern as a function of the RF frequency f taken at the spin flip probability ρ = 1 of the RF coils.

A special type of the amplifier was designed. The amplifier allows one an easy adjustment of the frequency in a wide range. The principal idea is to use the saw-like sequence of the signal in the amplifier instead of the sinusoidal one. The software of the SE setup was completely renewed in the MATLAB medium.

Thus the prototype of the setup for Four wave SE measurements has been built. In the next steps, the performance of the pi-flipper between the spin echo arms should be improved. The NRSE option of the SESANS should be realized at this setup.

Achievements

Task	Description / major progress	Partner
T19.2	Development of wide-angle polarization analysis in neutron diffraction and spectroscopy	CEA
T19.2.1	The on-beam polarization 80.2% was achieved and maintained constant within 2 days.	
T19.2.2	A new magnetostatic cavity allowing to achieve the magnetic life time of 3He up to 1000h in very large cells was developed.	
T19.3	Further developments of Larmor labelling methods for inelastic neutron spectroscopy	TUD
T19.3.1	Twelve crossed Pythargoras coils with thickness modulation and straight cuts each with an active area of 100x100 have been produced and are build in the J-NSE spectrometer in Garching and the SNS NSE spectrometer.	
T19.3.2	The TOFLAR instrument is simulated by Monte Carlo. For this purpose further developments of the simulation package McStas have been undertaken. A prototype has been built at RID, Delft..	
T19.4	Further developments of Larmor labelling methods for SANS and reflectometry	FZJ
T19.4.1	Theoretical analysis of the TGF spin-echo small-angle neutron scattering /reflectometer setup has been carried out. Special components for the VITESS simulation package has been developed and tested.	
T19.4.2	Several experiments using the MIEZE technique in combination with SANS measurements have been performed at instruments MIRA and RESEDA	
T19.4.3	A study has been made on spin flippers, where field flippers are distinguished in high and low field flippers.	
T19.5	Developments of wide angle neutron resonance spin-echo	TUM
T19.5.1	The thermal and mechanical stability of coils, the manufacturing and cooling technique are developed and tested on standard-sized NRSE coils.	
T19.5.2	NRSE coils with minimized amount of material: curved coils were designed and go in the testing phase at LLB and TUM.	
T19.6	Development of new polarized neutron techniques	TUW
T19.6.1	The ILL CRG-B instrument S18 may now be used routinely for USANSPOL measurements. Sample environment for characterization of magnetic samples under external magnetic fields and applied	

	mechanical stress was developed and is currently in prototype status. The instrument has been tested with various amorphous soft-magnetic ribbons with novel magnetostriction properties.	
T19.6.2	Numerical simulations of the polarization behind a resonator consisting of 18 separate current sheets have been carried out separated for three different beam cross-sections.	
T19.6.3	The prototype setup for the FW-NRSE experiments have been built. A special type of the amplifier allowing for an easy adjustment in a wide frequency range was designed.	

WP 20 MUONS

Objectives

Task 2: Technologies for high field instruments

Development of detector technologies and array designs, supporting the ongoing programme at both STFC and PSI to develop new muon instruments operating at magnetic fields of up to 10T.

Task 3: Technologies for μSR at high pressures

Development of pressure capabilities for μSR, both in the gas phase and for condensed matter; solving problems unique to μSR, such as the need for thin beam entry windows, positron exit and the provision of RF excitation.

Task 4: Novel resonance techniques and simulation codes for complex experiments

Development of the use of NMR-style pulsed RF techniques in μSR, including an in-situ NMR capability; development of simulation codes to aid analysis of complex μSR experiments.

Task 5: Muon beamline control and Modelling

Work to develop a better understanding of beam and instrument properties, including techniques for beam diagnostics and instrument simulation

Work progress

Task 1:

The website was launched (**D20.01**) following the 1st meeting of the JRA that was held earlier than anticipated to coincide with the NMI3/FP7 launch meeting (PSI, March 2009). This meeting provided a valuable opportunity for JRA partners to review the tasks included in the JRA, and commit to the timescales and deliverables associated with the project. The minutes were added to the website (**D20.03**). Discussion during the 2nd meeting of the JRA focussed on those tasks active during the initial 18 months of the grant period, with JRA members reporting on significant results and progress towards deliverables. This meeting was held to coincide with the 2nd General Assembly of the NMI3, and again the minutes have been posted on the website (**D20.13**).

Task 2:

Following the recent acceptance of the High-Field project at PSI, the final development of a High-Field detector system has begun well in advance of the anticipated date. A design for the final prototype has been finalized (**T20.2.1**) and the production is currently underway. A downgraded version with a reduced number of channels was successfully tested in December 2009 (**D20.09**), the achieved time resolution of $\sigma \approx 90$ ps was significantly better than the tolerable value of 140 ps. A prototype of the veto detector system, with scintillators at cryogenic temperatures and the readout using a lens system, was successfully tested in June 2010. Detailed design work for integration into the dilution refrigerator is under way.

System acceptance testing of the 5T longitudinal field magnet at ISIS was completed well in advance of the anticipated date, and muon beam experiments designed to assess system performance were concluded in Q3, 2010. Results are currently being assessed in preparation for a detailed report and journal publication describing system performance (**D20.14**) early 2011.

Dialog between the facilities concerning the development of high field techniques has been an important benefit of the JRA, with Dr. Scheuermann (of PSI) making a short visit to ISIS during Q4, 2009 to discuss aspects of the ISIS spectrometer performance with the Instrument Scientists (Drs. McKenzie and Lord). The recent high field workshop (Q4, 2010), organised by Drs. McKenzie and Hillier (ISIS), brought facility staff and users together at The Cosener's House in Abingdon, UK, to consider novel applications of high field muon spectroscopy.

Task 3:

Development of the solid sample pressure cell (**D20.25**) will start late 2010, and a PDRA has recently been appointed for this project. Some preliminary work has, however, already been carried out, with work at PSI focussing on computer simulations of the muon stopping range and signal (from sample) to noise (from pressure cell walls) ratio together with tests of a double-layer pressure cell.

Development of a gas-phase pressure cell (**T20.3.2**) is planned to start late 2010. Recent discussions with facility users have suggested that scientifically there would be considerable interest in developing gas pressure cells to work on the new ISIS high field spectrometer. As this fits well within the overall theme of the JRA, we propose refocusing effort for this sub task to provide ~50 bar gas cells for simultaneous high field and RF studies. The timescale will remain unaltered, with deliverables becoming (**D20.26**) 'gas pressure cell working within the ISIS high field spectrometer', and (**D20.28**) 'report on cell performance, including a demonstration of high field and RF measurements'.

Task 4:

Preliminary experiments have been carried out that have demonstrated the feasibility of applying NMR style pulse sequences to the RF µSR experiment (**D20.18**). Immediately apparent is the need for good RF engineering of the probes to ensure suitably intense pulses can be generated. To this end, an off-line test facility is planned to enable probe development to proceed without impacting on facility beamtime, and a dedicated high power RF insert is being designed for the ISIS high field spectrometer.

The development and demonstration of an in-situ NMR spectrometer is now complete and a report (**D20.08**) available on the JRA website. Good results have been obtained (**D20.07**) using both dedicated NMR coils and the RF cavities typically used for RF µSR experiments.

It is anticipated that this technology will find immediate application in the off-line test facility.

On June 22nd 2010 Dr. Tapas Samanta joined UNIPR as a PDRA for the sub task developing local muon field simulation software (**T20.4.3**). The skeleton version of the software, together with the scheme for its public documentation, available on a read-only wiki, has been planned. A few standard cases have been selected and successfully checked in a preliminary test version. A flow-chart of the intended implementation is included in deliverable **D20.02**.

Task 5:

With the need to evaluate the performance of the ISIS high field spectrometer during 2009/10, work within this task has focussed on developing the CCD beam camera (**D20.11**). The successful commissioning of the 5T magnet during 2009 enabled the camera to be tested in high magnetic fields during Q4, 2009, well in advance of the planned date. Excellent results have been achieved, with it proving essential to making the detailed performance evaluation of the ISIS 5T instrument required for **D20.14**. A report discussing the performance of the camera is available on the JRA website. With substantial effort being devoted to development of the camera the scheduling of deliverables within the period of the sub task 20.5.1 has been reviewed, with **D20.04** (a document assessing methods for providing better diagnostic information) being prepared Q4, 2010.

The simulation program '*musrSim*' (originally developed during FP6) has been extended, and has become a general tool for simulating almost any µSR apparatus (**D20.12**). It is currently being used at PSI for the development/optimisation of four instruments (the High Field Instrument (**T20.2.2**), LEM, ALC and GPD). At ISIS, Dr Bakule of the RIKEN-RAL facility has used the program extensively both in the development of the low energy beamline and as a means of understanding the operation of the ARGUS collimator, while it has also played a crucial role in the interpretation of a combined laser stimulation/µSR measurement made by Prof. Fleming (of the University of British Columbia). While '*musrSim'* is relatively simple to run, the analysis of the simulated results to a graphical output (histograms, µSR spectra, etc) still requires an analysis program to be coded specifically for a given instrument. A general analysis program, designed for an arbitrary setup of positron, muon, veto and coincidence counters, is currently under development.

Synergy between the tasks within WP20 is evidenced by the important role '*musrSim*' has played in the High Field project at PSI. The program well reproduced the measured µSR spectra at ALC and of the High Field tests carried out in Q4, 2009, thus giving great confidence in the design of the High Field instrument. Simulations not only enabled limits to be set on the dimensions of the cryostats, parameters of the High Field magnet, dimensions of the collimators, etc, but were also crucial in deciding which magnet, cryostat and spin-rotator to purchase.

NeXus files are now routinely used at ISIS, and work is underway to devise an upgrade of the Instrument Definition suitable for both ISIS and PSI facilities (**D20.21**). This definition will later be extended to include beamline parameters.

Achievements

Tasks associated with WP20 have progressed well during the first 18 months of the project, with the defined deliverables having been achieved. An early review of the project plan highlighted the need to delay Task 20.4.3 until a PDRA could be appointed; this appointment has now been made and the Task is in progress. Recent discussion with facility users have highlighted the scientific interest in developing ~50 bar gas cells for the ISIS high field spectrometer, and we plan to refocus this activity (due to start Q4, 2010) accordingly.

Task	**Description / major progress**	**Partner**
T20.2	Technologies for high field instruments	PSI
	T20.2.1: Appropriate timing resolution for the 10T detector system has been demonstrated (*D20.09*) and the prototype design finalised.	
T20.3	Developing technologies for µSR at high pressures	BBU
	T20.3.1: A PDRA has been appointed and preliminary design work carried out; *T20.3.2*: Recent discussions with users have highlighted an interest in developing gas cells for the ISIS high field spectrometer. This fits well within the overall theme of the JRA, and we propose refocusing effort to provide ~50 bar gas cells for high field RF studies.	
T20.4	Novel resonance techniques and simulation codes for complex experiments	STFC
	T20.4.2: Demonstration of an in-situ NMR spectrometer is complete and a report (*D20.08*) available on the JRA website; *T20.4.3*: A PDRA has been appointed and project planning completed. A document discussing the scope of the simulation codes (*D20.2*) has been completed.	
T20.5	Muon beamline control and modelling	STFC
	T20.5.1: A CCD camera for high field beam imaging has been developed (*D20.11*) and used to commission the 5T high field magnet. A general assessment of beam diagnostics will follow Q4, 2010; *T20*.5.2: The program '*musrSim*' has been extended to permit simulation of almost any muon apparatus (*D20.12*), and used extensively for instrument development and experiment analysis; *T20.5.3*: Work towards an upgrade of a NeXus Instrument Definition suitable for both ISIS and PSI facilities is underway.	

WP 21 SAMPLE ENVIRONMENT

Objectives

The principle aim of the JRA is to enhance the capabilities of sample environment available at neutron facilities. We will extend the supported sample environment at the participating facilities and provide knowledge and expertise to the collaborating participants. The three key areas of endeavour are high pressure gas cells, ultra high temperature furnaces and gas handling systems.

High Pressure Gas Cells

In the area of high pressure gas cells the aim is to increase the range of available pressures to 10 kbar (inert gases) and 8 kbar (hydrogen) and thus have a significant impact on the range of science possible. There is a need to design cells with adequate strength while allowing sufficient neutron transmission, and to provide safe and user-friendly gas handling systems to charge the cells for the beamline.

Considering the inert gas cells, the aim in this period has been to assess and review the current technology available; to hold a design plan review to formulate design ideas and address potential issues; and to begin the design and manufacture of a 8 kbar inert gas cell. For the hydrogen cells, development has been complicated by safety and material embrittlement concerns, thus research into suitable materials for cells is ongoing, and the pressures achieved have been lower: in this period a 4 kbar cell should be completed and the manufacture of a 6 kbar cell in progress. In the area of gas handling systems update work on the STFC hydraulic intensifier was planned and the start of the procurement process for a 10 kbar intensifier should be underway. The STFC should also be in the process of procuring a 8-10 kbar hydrogen handling system ready for testing prototype cells later in the project. The HZB have already acquired a 10 kbar hydrogen system and commissioning is planned. The CEA planned to procure a new cryogenic system for low temperature pressure tests.

High Temperature Furnaces

The study of structure and dynamics in liquid metals and dielectric materials is fundamentally significant and of important technological interest but is often prevented by the chemical reaction of the high temperature melt with its sample holder. The development of two types of levitation system will offer greater access to high temperature ranges for a wider range of materials.

The design and drawings of the aerodynamic levitation furnace were expected to be completed in this period. A meeting is planned to evaluate the design principles of the electromagnetic/static levitation furnace. This evaluation is the first step in the design of the sample position electrostatic systems and laser, to be completed late 2010.

Gas Adsorption Control Systems

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 aim of this task is to significantly extend the range of systems available to allow real-time in-situ measurements of many diverse chemical and physical phenomena.

In this period it is the intention to achieve significant progress in the development of a volumetric low pressure (<1.5 bar) gas adsorption measurement system for experiments in an Orange cryofurnace (1.5-600 K) and, alternatively, in a cryogen-free miniature pulse tube refrigerator (50-600 K). In addition the construction of a magnetic suspension balance for neutron environments should be underway, contributing to the completion of a magnetic gravimetric system.

Work progress

T21.2.1

In the “Report on current inert gas pressure cell technology” (D21.02) the high pressure technique based on gas medium compression has been investigated and reviewed. The report has been posted on the JRA Sample Environment website.

The 13.8 kbar oil intensifier system (D21.06) planned to be used for high pressure cell testing has been assembled and successfully tested up to 13.8 kbar. The intensifier is now fully operational and has been released to the user programme. The 10kbar inert gas system specification has been completed (M21.2.1.2) and the procurement of the system is underway.

A new top-loading cryostat required at LLB to cool down the pressure cells in a more convenient and reliable way (D21.07) has been designed and made by AS Scientific Products Ltd. Final delivery to Saclay took place in March 2010. Commissioning has been completed and the equipment was available to users for the reactor re-start in May. Good progress has been made with the design for the 8 kbar test cell and a design plan review (M21.2.1.1) has been held.

Figure 52: Top-loading cryogenerator at LLB. General view of the cryostat during testing at 20° tilt.

T21.2.2

The high pressure hydrogen gas cell for 4 kbar and up to 700K (D21.08) has been modelled, designed, manufactured and successfully tested at ISIS facility up to 500K. Testing to 700K will take place later in the year. The design and construction of a prototype 6kbar cell up to 300K (D21.24) is underway.

The HZB hydrogen gas handling system has been successfully commissioned (D21.03).

T21.3.1

After the discovery of a new and very promising, aerodynamic technique it has been decided to construct a test rig, nozzles of different geometries and a set of balls covering the densities and sizes of the samples that are expected to be investigated with the levitation furnace in order to aid the design process. The optimum gas flows to be injected in the two nozzles for the set of balls has then been determined.

The levitation process is very well controlled in the horizontal (scattering) plane but there are still some vertical oscillations under investigations.

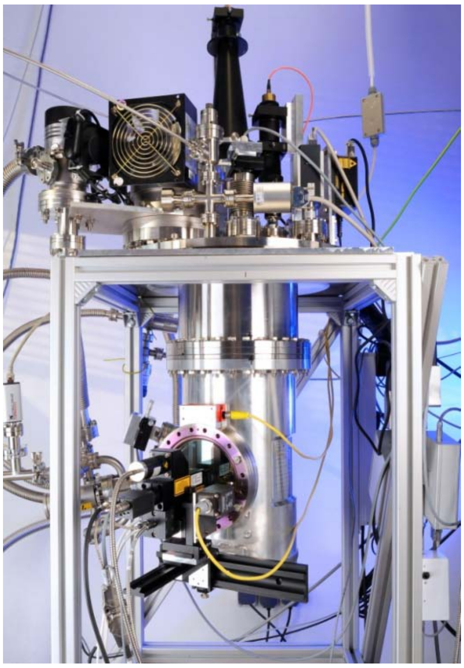


Figure 53: Electrostatic levitator for neutron scattering.

T21.3.2

Vacuum chamber parts of the NESL (Neutron Electrostatic Levitation) have been assembled and leak tests have been performed successfully. The assembly of the main components (as far as possible: some components are temporary) of the NESL has been completed. Constructional measures to meet safety requirements to avoid laser radiation hazards have been made (D21.10).

First test runs of the prototype NESL were performed successfully at DLR using known conductive samples. The remote control software has been tested. Further software adjustments have to be made. Problems arising with the UV lamp due to bad vacuum after sample change show the need of a sample change mechanism. The construction of a sample changer will be completed within the next month.

T21.4.1

The construction of a sample-stick for controlled gas adsorption experiments (1.5K – 600K) at pressures up to 300 bar and a pulse tube refrigerator for low pressure in-situ gas adsorption experiments in the temperature range from 55K to 320K is finished, with several options for sample cells **(D21.11)**. The design and construction of a 600K option for the pulse tube is in progress. Final testing **(M21.4.1.1)** and improvement has started.

Figure 54: Pulse tube refrigerator for in-situ gas adsorption experiments.

The software for the remote operation option of the 500K gas handling system **(D21.21)** has been implemented. The calibration of the pressure gauges at high temperatures has started. The basic software for the remote operation is implemented and will be extended to be used with a scripting language. Heated capillary tubes for “hot” external connections have been procured.

T21.4.2

The magnetic suspension balance system for neutron scattering **(D21.17)** has been improved for experiments with non-isotropic sample which require an exact repositioning of the sample (after weighing). The design of the high temperature extension up to 500°C is in process **(M21.4.2.1)**. A docking system for high accuracy humidity control based on saturated salt solutions has been developed which supplements the vapour mixing method **(D21.25)**. A draft design of the low temperature extension **(D21.33**) is finished.

Achievements

Task 21.2 – The delivery of the 8-10 kbar hydrogen handling system will be delayed until the end of 2011. This is because financial constraints have forced the STFC to build the system in house (D21.12).

Task 21.3 - The furnace design is still being discussed because of the problems encountered with the vertical oscillations and the production of the drawings is therefore delayed by several months. (M21.3.1.1 & D21.09)

Task 21.4 - We started work on tasks D21.11, D21.25 and D21.33 several months in advance because of the necessary compatibility with task D21.17.

Task	Description / major progress	Partner
T21.2	High pressure cells	STFC
T21.2.1	Gas handling & pressure cells for inert gases	STFC
	D21.02 Complete 1/12/09	

	D21.06 Complete 1/03/10 D21.07 Complete 10/03/10 M21.2.1.1 Complete 30/11/09 M21.2.1.2 Complete 01/10/09	
T21.2.2	Hydrogen gas handling & pressure cells	STFC
	D21.03 Complete 30/12/09 D21.08 Cell complete, tested to 500K 30/08/10	
T21.3	High temperature furnaces	ILL
T21.3.1	Construction of an ultra-high temperature aerodynamic levitation furnace	ILL
	D21.09 Expected 31/10/10 M21.3.1.1 Final review delayed	
T21.3.2	Ultra high temperature furnace using electromagnetic/static levitation	ILL
	M21.3.2.1 Complete 30/12/09	
T21.4	Development of Gas absorption Control Systems	HZB
	D21.11 Complete 30/04/10	

WP 22 DETECTORS

The aim of this JRA is the development of new detector technologies based on Gaseous Scintillation Proportional Counters (GSPC). These devices have the potential of improving the performance of high position resolution detectors used in reflectometry and time resolved SANS. Present state of the art detectors, such as ^{3}He-based Multi Wire Proportion Chambers already limit the performance of existing reflectometers due to their moderate count rate capability. They only provide limited spatial resolution of x ~1-2 mm and a time resolution in the microsecond range. More advanced devices based on solid ^{6}Li-doped glass scintillators with Anger camera readout, e.g. as recently developed at the SNS, can partially improve the performance achieving high position resolution (~1mm) and providing good timing resolution due to the fast scintillation light pulse with a duration of about 200 ns. The low light output of ^{6}Li glass however, diminishes the count rate capability due to the signal integration time required. A major drawback of ^{6}Li based glass scintillation detectors is a non negligible sensitivity to a high gamma background environment.
Micro pattern charge amplifying structures like MSGCs have been shown to be very efficient in the production of fast scintillation light in the visible region when operated in the proportional mode in gas mixtures of ^{3}He-CF_4. Photon yields per detected neutron can be ~100 times larger than that of ^{6}Li-glass and light signal durations of less than 60 ns have been observed. In the proposed JRA particular emphasis is therefore placed on the development and study of new technologies based on these Gaseous Scintillation Proportional Counters with light readout. The application of this new technology in neutron detection could enable the design of neutron counting detectors with superior performance that exhibit a high count

rate capability of up to 10 MHz, a high spatial resolution (~1 mm) and a low gamma sensitivity on a par with gaseous detectors.
The work will be organized in two tasks. The first task is concerned with the development of the GSPC based detector technology and the second task seeks to develop the related readout devices and electronics.
Task 22.2 will explore the perspectives of Gaseous Scintillation Proportional Counters based on ^3He-CF_4 gas mixtures at high pressure and various charge amplifying structures (MSGC, ITOMSGC, GEM) read out by position sensitive light detecting devices.
Task 22.3 will explore the light read out devices and the front end pulse processing and readout electronics for GSPC detectors. It is not the intention to construct a full sized detector within this WP, due to cost and time limitations. Instead, a number of different technologies will be identified and explored and their usefulness in achieving the desired range of specifications will be assessed. Based on this work a small scalable detector including readout electronics will be constructed during the course of the initiative. This will act as a demonstrator for full sized 20 cm 20 cm detector.

Task 22.1:

The JRA-22 start meeting was held as satellite of the NMI3 launch meeting at PSI on March 30. It was followed by the 2nd JRA meeting which was held at FRM II in Garching from 10-11 December 2009. It was attended by 17 participants from five partners. The 3rd JRA meeting again was held as satellite of the GA meeting in Bareclona on May 10. All presentations given at the meetings were put online on the JRA-22 website which has been launched together with the web-based forum in the period reported.

Task 22.2

This task will explore the perspectives of GSPCs based on ^3He-CF_4 gas mixtures at high pressure and various charge amplifying structures read out by position sensitive light detecting devices.

Hisako Niko and Luis Pereira (hired by ILL and LIPC respectively) at ILL presently study the physical fundamentals and the detector principles of a GSPC. In view of the applicability of different micro pattern devices for GSPC three different detectors have been built there.

A 20cm x 20cm large MSGC with 3 mm pitch and parallel charge division readout along the anode strips has been built and successfully operated with total gas pressure up to 5 bar. Designed for high rate capability the chromium anode strips are covered with an additional Aluminium layer to reduce the resistivity. A count rate capability >100 kHz /anode without efficiency losses has been achieved in a beam test and a position resolution of 2mm along the anode strips has been measured with the device operated at 2 bar CF_4 pressure. Under direct beam exposure the detector revealed irreversible ageing reducing the neutron pulse height by a factor of 2. This phenomenon not yet understood will be investigated with an improved device.

A 80mm x 80mm large MSGC 80 with 1mm pitch and “virtual cathode” layout (Schott glass S8900) equipped with a SUPRASIL quartz window has been built for primary and secondary light studies. Combined with an Anger camera arrangement of 4 EMI 9125A PMTs (bialkali photo cathode) it allows to determine the methods adequate to characterize the detector performance. A fast Aqiris digitizer readout system enables to study the time development of the light signal and the performance of different localisation algorithms. The detector is filled with 2bar ^3He and 3bar CF_4.

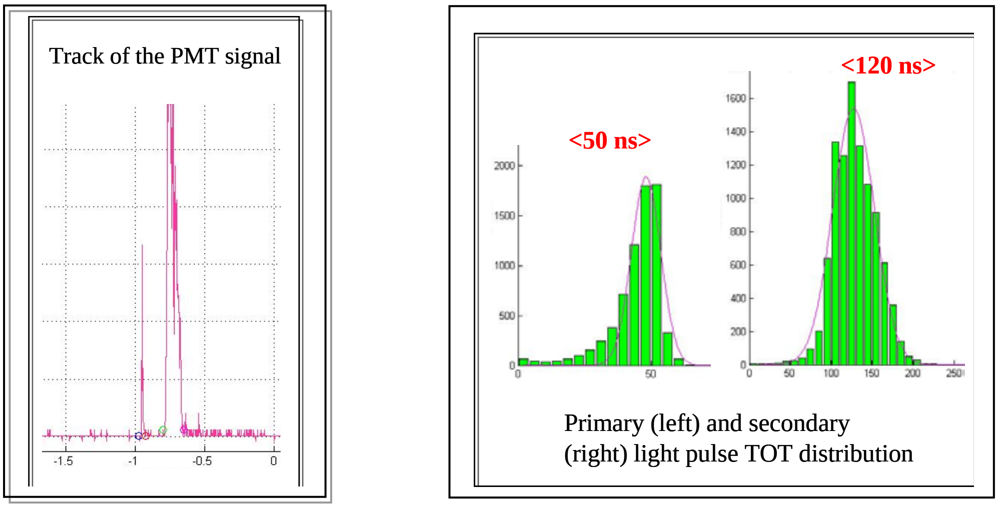


Figure 55: a) PMT signal track produced by a neutron; b) Duration of primary and secondary light pulse

Figure 55 a) shows a PMT signal track of a typical neutron event revealing the primary and secondary light pulse and b) the resulting distribution of the pulse duration of primary and secondary light which is determined in average to 50ns and 120ns respectively.

A 90mm x 90mm large MSGC 500 with 0.5mm pitch and standard single sided layout on S8900 glass has been built to compare its performance in a GSPC with the “virtual cathode” MSGC 80. It has been mounted in the same pressure vessel with identical mounting geometry. In a first test with neutrons however, it revealed a strongly deformed pulse height spectrum which is attributed to a non adequate mounting. After a redesign of the mounting the device will be investigated in a further beam test.

The yield of secondary photons per electron produced by a neutron in a GSPC drastically increases with the CF_4 partial pressure. The design study of an adequate pressure vessel capable of operating a GSPC at high pressure therefore is the second main task performed at ILL. A prototype has been designed and successfully tested up to 8 bar fill pressure. Equipped with a single PMT readout it allows to study light yield and signal speed as a function of fill pressure, gas composition and electric drift field. First preliminary measurements have been performed.

The emission of primary and secondary light in CF_4 scintillation is divided in two main components in the UV and the visible part of the spectrum respectively. At LIP absolute measurements of the spectral emission of primary and secondary light by CF4 have been performed in the fill pressure range 0,5 bar < p < 5 bar. The system was calibrated using a deuterium lamp in the UV and a tungsten lamp in the visible region. Figure 56 shows the resulting spectra of primary light indicating a strong dependence of the relative intensity of the UV and visible component on the CF_4 partial pressure in the absence of an electric field.

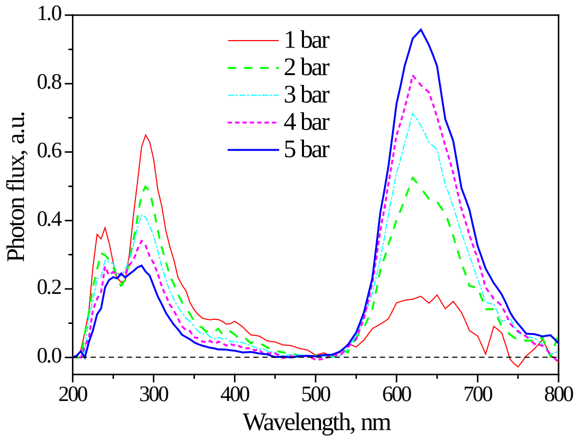


Figure 56*:* Spectra of primary scintillation light as function of CF4 partial pressure

In the same condition the effective live times have been measured to ~ 4 – 6 ns for the UV component and ~8 – 16 ns for the visible component. In contrary to the UV component the visible part shows clear pressure dependence.

Figure 57 shows the spectra of secondary light as function of CF_4 partial pressure. The spectral profile shows weak dependence on the CF4 pressure and is similar to the corresponding profiles of the primary emission in the presence of a strong electric field. From these spectra a photon-per-electron ratio of 0.035 has been determined for the secondary emission.

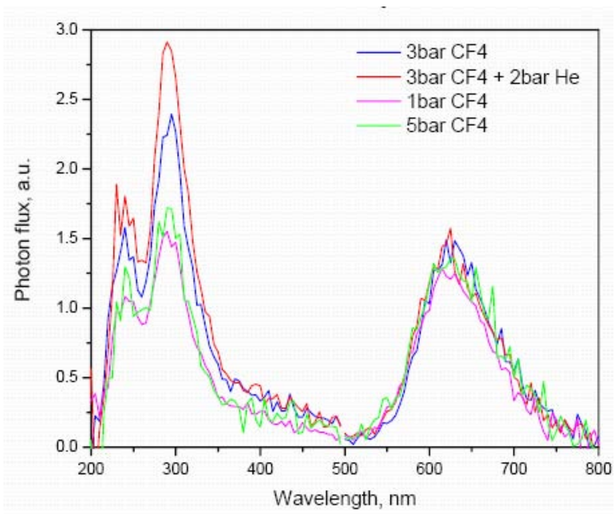


Figure 57: Spectra of secondary scintillation light as function of CF4 partial pressure

With the setup at LIP it could be shown that the presence of an electric field can drastically change the situation. While in view of the relative intensity of the UV and visible component no effect was observed for low CF_4 pressure a strong reduction of the visible and an increase of the UV component with increasing electric field is observed for medium – high CF_4 pressure. At 5 bar a strong reshaping of the UV component is detected. Regarding the effective live times again the UV component is hardly affected while the visible component shows a clear slowing down with increasing electric field at high CF_4 pressure.

The admixture of He showed no effect on the time evolution of the CF_4 scintillation but slightly increases the total intensity of emitted primary scintillation light. Additional admixture of small impurities of Nitrogen however, seems to strongly quench the emission of the visible component.

In course of the studies at LIP the photocathode uniformity of the employed Hamamatsu PMTs was investigated using a dedicated scanning system. Ten existing PMTs were scanned with 1 mm resolution and the resulting maps show that the relative sensitivity within each PMT can vary as much as 18%.

In March 2010 a workshop dedicated to data acquisition and signal analysis has been organized by Bruno Guerard at ILL. In particular, data analysis and Monte Carlo simulation software developed at STFC, LIPC and ILL was demonstrated and distributed to members of other facilities involved. Simulations have not progressed further. If the software distribution and training session doesn't fill the perceived requirements of the other working group members, STFC will conduct a review to list simulations required, in order of priority, and determine a suitable work programme. Davide Raspino from STFC will be available to carry out simulations, experimental development work and analysis.

Task 22.3

This task will explore the light read out devices and the front end pulse processing and readout electronics for GSPC detectors. The partners involved (FZJ, STFC, TUM) have agreed upon the construction of a "standard GSPC-light source" for the study of different light detecting devices. Based on prototype devices developed at LIPC and ILL in the course of the previous MILAND programme three identical detectors have been designed and built at FRM II and have been distributed among the partners after mechanical and functional tests at FRM II. Based on a common MSGC design (ILL6C on D263 glass) for light production, the device will easily allow a comparison of different light detecting devices investigated at the individual labs.

In April 2010, the first of three devices has been investigated at TREFF test beam facility at FRM II operated with 1 bar CF_4 + 0.3bar ^3He filling and a SUPRASIL quartz window. The "light source" could be equipped with three different light readout systems.

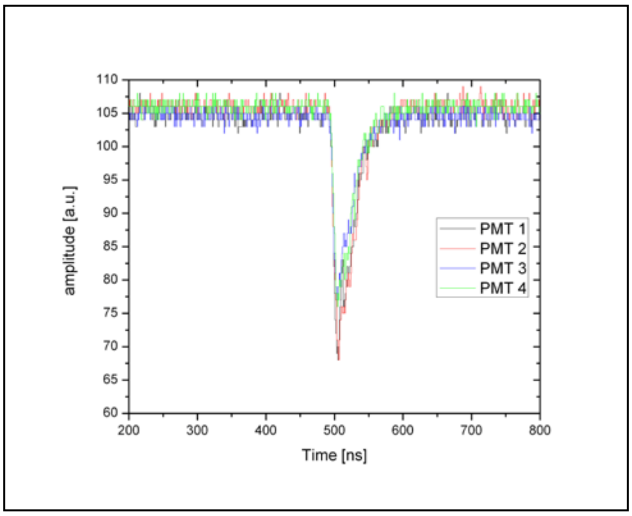


Figure 58: PMT signal tracks of the FZJ 4-PMT Anger array produced by a neutron

A single Hamamatsu H1949-50M PMT (bialkali cathode) was used to study the signal development of primary and secondary light pulses produced by neutrons.

An Anger camera arrangement of four ET Enterprises 38 mm PMTs with glass window and bialkali photocathode built at STFC could be mounted for position algorithm studies. At STFC, six of these PMTs had before been evaluated for gain similarity and equipped with their corresponding negative polarity voltage divider networks.

An Anger camera arrangement of four Hamamatsu 38 mm PMTs with glass window and bialkali photocathode built at FZJ could be mounted for comparison. Five of these PMTs had before been evaluated for gain similarity and equipped with their corresponding positive polarity voltage divider networks at Jülich.

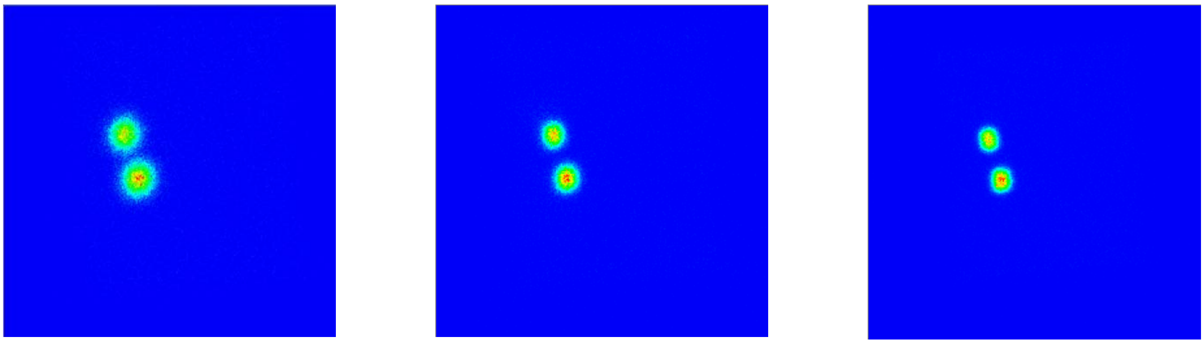
All readout devices were recorded using an Aquiris digitizer system meanwhile available in each participating lab. As an example Figure 58 shows the four single PMT signal tracks of the FZJ Anger array produced by a neutron event when the detector is illuminated in the centre with a collimated beam.

Aqiris capture and visualisation programmes developed by STFC during MILAND have been modified to operate with Aqiris systems of other working group members. These programmes were demonstrated and distributed at the ILL workshop.

The device delivered to ISIS has been filled with 1 bar ^{3}He and 2 bar CF_4. It was equipped with four 38 mm diameter red sensitive PMTs from ETL. These PMTs have UV windows and are able to detect, with reasonable efficiency, photons from the CF_4 emission lines at 300 nm and 650 nm. An initial position resolution of 1.5 mm has been obtained for the detector. The effect of increasing voltage on the PMTs and the microstrip has been explored. Figure 59 shows the image of two 0.5 mm diameter holes in a cadmium mask as a function of microstrip anode HT. The position resolution improves in going from 850V (gain ~5) to 1000 V (gain ~10), but hardly changes when the HT is raised further to 1180 V (gain ~50). The results show that the detector resolution is not limited by the gain of the microstrip. Similar results show that the PMT gain is also not limiting detector resolution and the most significant factor is probably the CF_4 pressure.

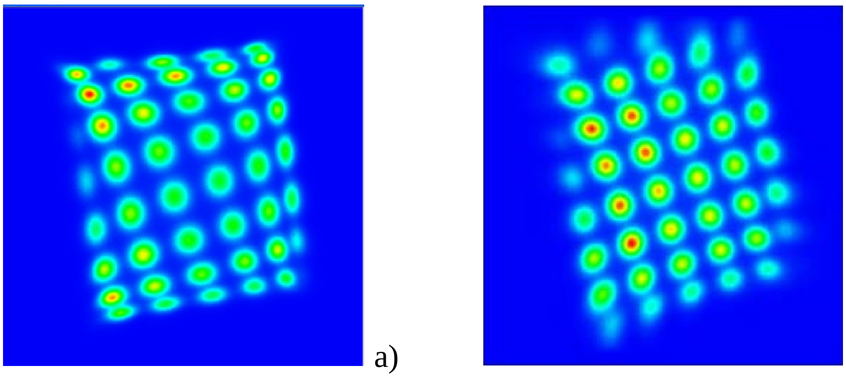
The full field of view of the microstrip has also been explored, Figure 60a) shows an image of an array of 2 mm diameter holes in a cadmium mask and b) shows an initial reconstruction of the image which corrects for detector edge distortion.

This device is working extremely well and provides a vital aid in optimising choice of PMT and development of PMT and signal processing electronics in the next phase of the project.



a) *b)* *c)*

Figure 59: Images of two 0.5 mm diameter holes on a 5 mm pitch in a cadmium mask with the microstrip anode at a) 850 V, b) 1000 V and c) 1180 V



a) b)

Figure 60: Image of an array of 2 mm diameter holes on a 5 mm pitch in a cadmium mask a) uncorrected and b) corrected for edge effects

CNR addressing innovative light detecting devices has started to build a small Si-PMT based prototype device. A SiPM produced by IRST (Trento, Italy) with 3 x 3 mm^2 effective surface has been coupled to a proper (not integrated) front-end electronics and preliminary tests using ambient light have been successfully performed to estimate the gain. First estimate by evaluating the response from fixed number of photons confirmed the expected performance of a gain of about 10^6. After successful tests in the lab the device has been coupled to a 1 mm thick GS20 Li-glass and a 300µm thick ^{6}LiF/ZnS scintillator and its performance was investigated in two experiments performed with λ = 4.7 A neutrons at the TREFF test beam facility at FRM II.

Achievements

Task	Description / major progress	Partner
T22.2	Gaseous Scintillation Proportional Counter	ILL
	At ILL two prototype detectors based on different type of MSGCs have been designed and produced and serve for the study of primary and secondary light emission characteristics in CF4 based GSPCs. In addition, a third device capable of high pressure operation has been designed. After approval first measurements have been started. At LIP spectral shape and absolute intensity of the emission of primary and secondary light in the UV and visible range have been determined as function of CF4 pressure and electric field.	
T22.3	Light detecting devices and related front end, pulse processing and readout electronics	STFC
	Three identical prototypes serving as "standard" light source for the study of different light detecting devices have been produced and distributed to the partners involved. First preliminary tests using various types of PMTs have been performed at STFC and in a joint campaign of all partners at FRM II. CNR has built a small Si-PMT based prototype coupled to a 6LiF/ZnS szintillator or to GS20 glass and investigated its performance in a beam test at FRM II.	

2.2 *Project management*

Management (WP1) & Networking (WP2)[13]

Objectives (WP1): Coordination of the consortium and running of the central management team. This implies

a. monitoring of project progress and implementation in close collaboration with the NMI3 General Assembly and the NMI3 Board
b. consulting and managing the NMI3 Scientific Advisory Committee
c. Managing all aspects of the NMI3 finances, including the control and distribution of funds and the collection of financial statements
d. Liaising with the project officer of DG-XII in Brussels
e. Publicizing NMI3 via appropriate publications and by providing the Information Services Manager with the relevant input (see WP3).

Objectives (WP2):

f. Organisation of the first and second NMI3 General Assembly with all Joint Research Activities.
g. Organisation of the first NMI3 Advisory Committee meeting
h. Organisation of NMI3 management and work package coordinators business meeting

Results (WP1&WP2):

The management team organised the launch meeting end of March (March 2009) (first general assembly and first board meeting). They set-up the scientific advisory committee sent out invitations to membership. These three organs of the project are accompanied by the revision of the address databases and the forums on the Neutron Portal.

The advance payment was received in March by the coordinating facility and completely redistributed to all beneficiaries in April as agreed during the board meeting.

They follow-up of the project schedule will be done with MS Project and staff was trained for that purpose. This allows also to plan the next proposal directly with this software.

Set-up of all the instruments and internal administrative rules (time record policy, reporting procedure, meeting schedule etc.) to guarantee sound project management.

Networking meeting with other I3 project coordinators was held on April 21st in Frankfurt.

The coordinator represented NMI3 in Prague on the European Research Infrastructures Conference in March 2009 and as well in Barcelona on the ECRI meeting in May 2010.

The information manager presented NMI3 at the ICNS in the USA on May 3rd -5th, where a collaboration with other international neutron user communities was discussed and agreed on (US user community and ANSTO). She was also presenting NMI3 with a booth at the SNI2010 in Berlin (February 2010) and at the GENESYS meeting in Barcelona in May 2010.

In 2010 the second general assembly was organised in Barcelona with the help of the Spanish user community representative (May 2010). The first scientific advisory committee was held prior to the assembly (feedback see D2.2.1)

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[13] WP1 and WP2 are closely related so it seems more coherent to present their results together.

The contact with the scientific officer is held in a regular manner, via phone and mail. And it is agreed that he will receive the minutes of business meetings, as his budget and time would not allow attendance to all NMI3 meetings.

Coordinators also travelled to Brussels (May 26th, 2010) in order to discuss the requirements for the first report, the future requirements for the transnational access activity and possible improvements.

The project manager followed a three day practical training on FP7 financial issues in order to be best prepared for the first reporting.

One head of facility meeting was organised in order to prepare the next proposal (summer 2010), over 20 expressions of interests were collected prior to the meeting (June, 29th, 2010)

Claim input for the internal monitoring reports as well for the first periodic report with its form C and evtl. certificates of financial statements (CFS). Till now one internal monitoring report at month 6, a rehearsal periodic report at month 14 and finally the first periodic report were established.

Regarding the future development of a common user access portal and the TAA support by the Commission, an Access Working Group (AWG) was created and the Access activity coordinator was confirmed in the second Board meeting in Barcelona 2010. Possible interactions with other EU projects like e.g. EUROFEL or national initiatives like HDRI (High data rate initiative) by the Helmholtz Gesellschaft in Germany were discussed. A common objective is to benefit from synergies instead of having several standards.

Dissemination (WP3)

Objectives:

a. Dissemination of the project and its results, and of other closely related activities in European neutron scattering and muon spectroscopy, predominantly through the European neutron/muon portal (web site)
b. To plan for the future through a regular series of foresight studies
c. Training activities to improve effective use of neutron and muon facilities via call for proposals, support to the well known „Hercules‟ course, in collaboration with the x-ray I3.
d. Web based training material, aimed at both university students and new facility users, utilising „virtual instruments” .

Results:

a. The I3 initiative to create a “Research Infrastructure” brochure targeting the large public was a large success and highly supported by NMI3. The highlights presented in the brochure with link to NMI3-FP6 where thoroughly chosen and edited by a scientific editor.

   Two articles were published in the Neutron Magazine (launch meeting, ICNS) in Vol.20, Iss.3 in September 2009, two other articles on web 2.0 and on women in neutron science are published in Vol.21, Iss. 3 in September 2010.

   The Notiziario has published an article on the second general assembly in 2010.

   The NMI3 management team met the Neutron News Editor Herma Buttner to discuss future plans and collaborations: next NMI3 advertisements on the back page of the magazine, education articles and coordination of reporting on events supported by NMI3.

   Two work-meetings with the information manager for future development of the web site (Neutron Portal) and new communication strategies in order to reach new neutron users and the broad public.

The server hosting the web portal was relocated from NetCologne to FZJ, where sustainability can be assured through support and maintenance by the FZJ IT staff.

EU project factsheet for NMI3-FP7 was edited.

Several responses to questionnaires for EC inquiries or other EU project inquiries (e.g. Cordis site, I3 PP comparison).

Several new communication materials were designed (e.g. NMI3 roll-ups for conference booths with a little logo contest and book prizes, Ultra Cold Neutron cubes as give away, Newsletter etc)

b. A foresight study for ESS Long-Pulse Instrumentation was held in August 2009 in Italy. Two more were planned for autumn 2010.

c. Four calls for proposal were launched for neutron and muon training activities:

   First call (early 2009) – 14 proposals received and 8 retained for funding (40K€ plus 30K€ for Hercules);

   Second call (summer 2009) – 14 proposals received and 6 retained for funding (30K€);

   Third call (early 2010) – 9 proposals received and 6 retained for funding (28K€).

   Fourth call (summer 2010) – 2 proposals received, both retained (7.5K€)

d. A new educations corner was set up and is under continuous improvement, as training material is uploaded via a wiki-media software solution.

NMi3 Meetings:

Date	**Venue / Organiser**	**Topic of meeting**	**Who participated**
30.03.2009	Villigen, PSI	NMI3 Launch meeting	all
30.03.2009	Villigen, PSI	JRA meetings	WP20, WP21, WP22
24.02.2009	Grenoble, ILL	JRA meeting	WP18
20.04.2009	Delft,TU	JRA meeting	WP19
08.10.2009	Graching, TUM	Business meeting NMI3	All WP coordinators
09.10.2009	Garching, TUM	JRA work meeting	WP18
29-30.10.09	Saclay, LLB	Sample environment	WP21
10-11.12.09	Munich, FRM II	Detector meeting	WP22
22.02.2010	Paris	Wide-angle polarizers (WAPANS)	WP19
17.03.2010	Alpe d'Huez	Monte Carlo Simulation meeting	WP16
03.05.2010	Abington	Data Analysis networking meeting	WP16
10-12.05.10	Barcelona	2nd General Assembly + 1st Scientific advisory committee	all
29.06.2010	Geesthacht, GKSS	Head of facilities meeting	H. Schober, M. Förster +Board representatives

External event with NMI3 presence:

Date	Venue / Organiser	Topic of meeting	Who participated
April 2009	Prague	ECRI 2009	H. Schober
21.04.2009	Francfort	I3 networking	H. Schober, M. Förster, A. Claver
May 2009	Knoxville, USA	ICNS	A.Claver (information manager), R.Rinaldi (SAC member)
18.06.2009	Copenhagen	FP7 workshop	M. Förster
August 09	Rome	Long pulse instrumentation foresight study	H. Schober, R. McGreevy
2009	Australia	ANSTO meeting	ENSA (A. Deriu)
Feb. 2010	Berlin	SNI	A.Claver
10.03.2010	Paris	French Ministry for Research infrastructures	H. Schober, M. Förster, Ch. Alba-Simionesco, S. Gota-Goldman, F. Leclercq-Hugeux
22-23.03.10	Barcelona	ECRI 2010	H.Schober, M. Förster
25-26.03.09	Grenoble	HERCULES 20th anniversary	H. Schober, M. Förster
March 2010	Alpe d'Huez	NOP 2010 International Neutron Optics Conference	P. Bentley, R. Cubitt, U. Filges, J, Fuzi, A. Ioffe, T. Krist, K. Lefmann, P. Mikula, F. Ott, L. Sani, J. Stahn, R. Valicu, P. Willendrup
April 2010	San Francisco, USA	MRS 2010	H. Schober
May 2010	Barcelona	GENESYS	A.Claver
26.05.2010	Brussels, EC	Meeting with officers	H.Schober, M. Förster
June 2010	Brussels	Financial Helpdesk workshop	M. Förster

2.3 *Access Activity*

Facility's words

ISIS – Science and Technology Facilities Council, Rutherford, UK

ISIS-Muons

The uniqueness of the ISIS Muon Facility means there is strong interest from researchers outside the UK. There is a well-established, experienced and dynamic European muon community who have developed and exploited the ISIS muon facilities since their conception. The experimental infrastructure of the Facility was constructed under funding from EC Framework Programmes 1 and 3 together with EC partners, and the Facility has run successful Access contracts under Framework Programmes 4, 5 and 6. Therefore, it is essential that the access contract continue which will allow European users from outside the UK to have access to the only pulsed muon facility in Europe.

To-date under the FP7 Access contract, researchers from 7 EC countries have been supported for 9 experiments to use the ISIS Muon Facility. 24 separate scientists have visited the facility to perform 9 different experiments. Of the 24 researchers who have visited, 13 were new users who had not used the Facility before FP7. These include new research groups (for example, new groups from Poland, Austria and Slovakia), together with doctoral students using the Facility for the first time.

ISIS-Neutrons

ISIS provides neutron instruments which give unique information on the structure and dynamics of condensed matter at the atomic and molecular level across a broad range of scientific fields, from physics and chemistry, through biological and material sciences to earth sciences, pharmacology and engineering. During this reporting period the ISIS Second Target Station has come on-line, providing a new set of state-of-the art instruments offering an enhanced flux of long-wavelength, low-energy neutrons for studies in areas such as soft matter, advanced materials, bio-molecular systems and nanoscience. The first publication from TS-2 was from an EU-funded experiment and appeared in Physical Review Letters in late 2009. In addition to new instruments, TS-2 offers new support laboratories and advanced sample environment equipment.

Providing access to these facilities to enable European researchers to fully exploit them for their research is very important. The Access programme provides funds which enable researchers to use ISIS who otherwise would not be able to. For the researchers, this gives them access to state-of-the art neutron instrumentation together with the excellent scientific and technical support provided by the facility which enables them to gain the most from their experiments. Demand for EU funding for experiments is very high - the programme at ISIS is many times over-subscribed, with far more requests than can be supported with the limited funds available. For the facility, the Access programme increases the quality and diversity of the scientific programme. This enables new science, and stimulates new collaborative activity for both scientific projects and for instrument developments.

During the first 18 months of the ISIS neutron FP7 access programme, 35 experiments have been completed and a further 5 have been allocated time. These experiments include Principle Investigators from 15 different countries (Portugal; Poland; Ireland; Austria; Romania; the Netherlands; Germany; Greece; Belgium; Italy; Spain; France; Denmark; Sweden; Slovakia). From the 35 completed experiments, 82 separate user visits have been made to ISIS by 69 individual users, 26 of whom were new users to ISIS. EU-supported experiments fall into the areas of energy, health, materials science, engineering and life science as well as fundamental studies.

FRM II – Technische Universität München, Germany

Right from the beginning of routine operation in 2005, about one third of the beam time available via our proposal system has been requested by European users. This strong demand could only be satisfied by the support within the NMI3 access programs in FP6 and FP7. The international collaborations and contacts promoted by the NMI3 program ensure a highly respected user program at the FRM II and enable us to compete with international leading institutes. The user beam fee is entirely used to hire additional stuff supporting the scientific usage of the neutron scattering instruments. This funding is of eminent importance for our institute to ensure a flexible personnel policy in order to meet the requirements of our scientific customers.

The limited resources in the running FP7 program, however, are exhausted already after 11 month by the end of the year 2009. The constraint through this limitation in the total budget caused right from the beginning of the FP7 program a reduction for travel support to only one scientist per experiment which especially harms the promotion of young scientists and students. As declared by our European users, the realisation of an experiment at the FRM II requires indispensable the support for travel and subsistence.

Whereas the most users are from countries with own neutron sources like France, the United Kingdom and Switzerland the other about 50% originate from 22 different countries. This indicates the wide spread of our international user community. Physics is still the dominating scientific area with the strong focus on solid state physics. Other important fields are materials sciences and engineering. Please find below a list showing the distribution of delivered days at the FRM II according to the scientific field of the projects.

JCNS – Forschungszentrum Jülich, Germany

Since the implementation of the I3 infrastructure programs in FP6 the Forschungszentrum Jülich GmbH has participated and extensively offered access to the European users. In 2006 the Jülich Centre for Neutron Science with Outstations at FRM II in Garching, Germany, ILL in Grenoble, France and SNS in Oak Ridge, USA was created to serve the scientific community with dedicated instrumentation in neutron scattering and strengthen the in-house research activities at Institute of Solid State Research at Forschungszentrum Jülich GmbH.

The I3 infrastructure programs have multiply proven to be of essential importance both for the users and for our facilities. There is a steady increase in the number of proposals and the numbers of users and user visits since the implementation of the programs. With the closure of the FRJ-2 neutron facility at Forschungszentrum Juelich GmbH in 2006 and the creation of JCNS and implementation of a suite of neutron instruments by JCNS at FRM II the interest and amount of users has further increased. The majority of the European users groups applying for beam time at JCNS would be unable to travel to JCNS without the option of financial support provided by NMI3

NMI3 has developed as a versatile tool for managing the facilities since the beam fee system provides flexible and highly efficient means to improve and enhance the user support from the facility point of view. The funding for investments (e.g. sample environment equipment, improvement to the instrument infrastructure etc) or for manpower (e.g. hiring PostDocs as instrument scientists) enhance in a unique way the attractiveness of the facility to the scientific community. It must be stated clearly that the participation in NMI3 provides an indispensable direct advantage both for the users and for the facility.

During the first 18 months of the project JCNS delivered 159 beam days to the users within NMI3. 34 eligible projects were supported. 27 individual users from 12 different European countries received financial support by T&S funds. Already within the first half of the supporting period of TAA JCNS has delivered more beam days to eligible users as contractually obliged demonstrating the demand and success of NMI3 in the scientific community.

A list showing the distribution of delivered days at JCNS according to the scientific field of the projects please find below.

SINQ – SμS, Paul Scherrer Institut, Villigen, Switzerland

The Paul Scherrer Institute operates three major user facilties on one campus: The Swiss Light Source (3rd generation synchrotron source), the Swiss spallation neutron source SINQ and the Swiss Muon Source SμS. Both SINQ and SμS (as also SLS) run open access user programs with 13 (SINQ) and 6 (SμS) instruments in full operation and a total of approximately 1000 user visits each year. The beamtime allocation is entirely based on a proposal system with two submission deadlines each year for both facilities. The proposals are evaluated during a peer-review selection process by international external selection panels that apply criteria entirely based on scientific merit. The total share of users from European countries is in the order of one third (SINQ) and even 40% (SμS).

During the first 18 months of the project SINQ and SμS delivered a total of **434** and **184** days to the users within NMI3, respectively. 73 (SINQ) and 35 (SμS) projects were supported and a total of 109 users were supported by T&S funds. At both facilities most of the funded proposals were submitted by British and German groups, followed by user groups from France. In total the delivered days were distributed among projects from 15 (SINQ) and 9 (SμS) different countries.

As in previous access programs we again delivered many more days to our eligible users than we were contractually obliged to deliver. This is a voluntary effort to strengthen the European user community, which is partly financed by PSI own funds. All those projects are reported in the MS Access Database but because of limited EC funding only part of those costs will be claimed.

Since the implementation of the I3 infrastructure programs in FP6 and even before both PSI neutron and muon facilities SINQ and SμS have participated and extensively offered access to the European users. The programs have multiply proven to be of essential importance both for the users and for our facilities. The numbers of users and user visits have doubled with the implementation of the programs and have stayed on that level stable ever since. This fact clearly documents the meaning of NMI3 for the users: Many user groups – in particular from universities - would be unable to travel to facilities like SINQ and SμS without this kind of support.

On the other hand NMI3 plays an essential role for managing the facilities since the beam fee system provides flexible and highly efficient means to improve and enhance the user support from the facility point of view. The access providing facilities are free to use the funding for investments (e.g. sample environment equipment, improvement to the instrument infrastructure etc) or for manpower (e.g. hiring PostDocs as instrument scientists). In our case, a couple of positions are funded by the available beam fees. Those are entirely used to improve the user support (e.g. hiring second instrument responsibles). Without that funding the user support at both SINQ and SμS would suffer significantly. Hence one can clearly state that the participation in NMI3 provides a win-win situation both for our users and for the facilities.

BENSC – Helmholtz Zentrum Berlin, Germany

The HZB (former HMI) operates a comprehensive user program at its research reactor BER II since 1993. 70% of the beam time at 14 instruments are offered to external users. The beam time allocation is based on a proposal system with two proposal rounds per year. The proposals submitted by external users are peer-reviewed by an international Scientific Selection Panel. Following the recommendations of this panel, the successful proposers are invited to perform the proposed experiments at the BER II free of charge.

From the beginning a high proportion of the external users of the BER II instruments came from EU and associated states. In the first 18 months of the present NMI3-FP7 program this quota was again about 50% as in former years. 630 beam days were delivered for 83 projects performed by 173 users from 17 different European countries (additional 6 visitors using 13 beam days for 3 projects at the end of the present reporting period are not yet taken up in the data base). These users were supported by the present access program. One third of them were diploma and thesis students. Usually they get only very restricted financial assistance for travelling by their home institutes if at all. It is solely the support provided by the NMI3 Access Program which enables them to visit one of the few neutron sources distributed over Europe and pursue their scientific projects.

The large number of external and in particular young and less experienced users imposes a high burden on a neutron facility (less than one half of the EU users of HZB declare themselves as experienced). To guarantee an optimal scientific output extensive expert support by in-house personnel must be provided. This is especially true when the experiments are performed under extreme sample-environment conditions (highest magnetic fields, lowest temperatures, controlled gas atmospheres etc.). Such experiments are the hallmark of the HZB. Here, the beam fee system of the NMI3 program provides a most valuable, flexible tool for compensating the extra efforts of the facility by allowing one to hire the additional personnel needed for the extended user support. At HZB the beam fees have always almost exclusively been used for this purpose. Only thus it was possible to maintain the high standard of technical and scientific support for external users, in particular for experiments under extreme conditions. The predominant part of the travel and subsistence support for EU users was instead taken from institutional funds of the HZB. These funds also allow us to support all EU-eligible visitors in the same way and not only those using the contingent of 240 beam days, the minimum amount of access foreseen by HZB in the present program.

LLB – Commissariat Energie Atomique, Saclay, France

LLB has been recognized as a "Large Scale Facility" by the European Union in the framework of the Human Capital and Mobility (1992), Training and Mobility of Researchers (1995), Improving Human Potential (1999), 6th and 7th (2003 and 2009 respectively).

This has made possible to receive a considerable number of individual European users (more than 450 since 1993). Up to now, more than 300 publications have come from the experiments supported by the HCM, TMR-LSF, IHP, FP6 and FP7 programs.

In the framework of the NMI3-FP7 Access Activities, 22 world-class neutron scattering spectrometers are opened to all scientists from European and Associated States. The travel and living expenses for usually two scientists per selected experiment are granted. Upon consultation with LLB, the stay at our Laboratory can be extended for preparation of experiment and/or data reduction.

The present LLB NMI3-FP7 Access program started the 2nd February 2009 for a period of two years and the LLB is required to provide 200 beam-days. However, the number of days the LLB is able to offer to European users is significantly higher. This is the reason why in this first 18 months-period, the LLB has actually provided 257 beam days. This is a voluntary effort to strengthen the European user community and to permit that groups form Universities (especially from countries having no national facility) could come to the LLB for performing neutron experiments. Many user groups would be unable to travel without this kind of support. The beam time is financed by LLB own funds. All those projects are reported in the MS Access Database but only part of those costs will be claimed.

The access beam fee returns 670588 € to the LLB for a period of two years. The most important part of the funding is mainly devoted to the improvement to the instrument infrastructure, in order to maintain the world-class of the neutron spectrometers opened to the ACCESS program. A part of this funding has been used to hiring two PostDocs for improving the user support and also to reinforce the User Office.

In particular, the ACCESS fees help us to upgrade the two hot neutrons spectrometers at the LLB, namely 5C1 and 7C2. At present there are only two hot sources available in the world, including the one at the LLB. These two spectrometers present and important overloading, and the number of European proposals are particularly high. Since hot neutrons provide unique access to large Q, it is our duty to equip our hot beam channels with the state of the art spectrometers. Therefore two of them 7C2 and 5C1 will benefit of major upgrade. Our liquid and amorphous diffractometer 7C2 will be equipped by new detector bank. Localization electronics, 256 position sensitive detectors and mechanics have been purchased and should be delivered by the end of the year. With its large, high efficiency detectors, the new 7C2 should have its counting rates increased by a factor of more than 20 in 2011.

GeNF – GKSS Forschungszentrum Geesthacht, Germany

The Geesthacht Neutron Facility (GeNF/GEMS-N) is operated as part of the German Engineering Materials Science Centre for research with photons and neutrons (GEMS) by the GKSS Forschungszentrum Geesthacht GmbH near Hamburg, Germany. The neutron source of GeNF/GEMS-N is the 5 MW swimming pool type reactor FRG-1 providing an unperturbed flux of 1.4×10^{14} neutrons/(cm^2s). About two thirds of the beamtime at the FRG-1 is provided to external users (typically 150-200 per year) from universities, research organisations and industry. Nearly half of the external use is focussed on engineering materials science (including biomaterials), the rest is split between physics, chemistry, biology and geoscience.

This research program will be kept up until mid of 2010 when the operation of the reactor is terminated. The research and user activities of GeNF/GEMS-N will then exclusively focus on the instrumentation build and operated by the GKSS outstation at the FRM-II.

Since the FP6 I3 programs the European users of GeNF profit from the support which is given by NMI3. It is a significant contribution to the use of the FRG-1 and enabled many users from a variety of European countries to visit GeNF. Without this support it would have been difficult to serve more than 100 students and experienced researchers from abroad.

In the year 2009/2010 from the EU-users 13 proposals were submitted to GeNF. In addition 6 approved proposals from 2008 were shifted into 2009. This adds up to 146 days of EU-beamtime which is 2.4 times more than the NMI3 funded beamtime days of 62 in 2009/2010. Due to our thorough pre-submission discussions between users (especially new users) and our beamline responsibles no EU-proposal was completely rejected. From the approved EU-proposals 16 were measured in person, two groups sent their samples. One approved experiment was cancelled because of the volcano eruption on Island in spring 2010. In sum 111 days of beamtime for EU users were delivered in 2009/2010. This is 1.8 times more than supported by NMI3 and reflects the high demand of neutron beamtime especially among European users from the European user community we had guests from Austria (34%), Netherlands (17%), Sweden (17%), Hungary (8%), Portugal (8%), UK (8%), Norway (4%), Slovakia (4%). The number of female scientists decreased to 31%. The speciality of GenF is the support of new users or users with no experience in neutron scattering. We were able to acquire 33% of new users in 2009/2010.

BRR – Magyar Tudomanyos Akademia KFKI, Budapest, Hungary

BNC has participated in the Transnational Access Programme from the FP5. A significant development occurred in BNC's access program when BNC joint to NMI3 in FP6. We could adopt high standards in our operation which have already been introduced in the large NMI3 partners. The proposal system and services provided to the users were improved and the result of this progress was the number of proposals increased significantly. The number of users visiting BNC facilities has been doubled and has remained that level during the fulfilment of NMI3 FP6 and FP7. The majority of BNC users are coming from the CE region, without NMI3 fund they could not afford to travel and carry out experiment on BNC facilities. We can state, that the implementation of NMI3 is essential for the users and also for the facility. It is essential for us, especially as a small partner of NMI3, that the beam fee can be used flexible; in our case the larger part of the beam fee goes for instrument and infrastructure developments (e.g. changing electronics, or replacing instruments parts, renovation of the cold neutron guide hall), and the smaller part contributes to the reactor operation. We would consider (in the next NMI3 project) using a part of the beam fee for hiring instrument scientist and additional staff to enhance the user services.

During the first 18 months of NMI3 project BNC has delivered 155 beam days. From the 30 eligible proposals 22 projects were supported and carried out by 27 users. From them 22 users could be supported with NMI3 T&S fund. The user statistics confirms BNC's regional role; almost half of the users came from the CE region including 4 countries while the other half came from 8 European countries, see the list of users.

As in the previous EC programs (FP5, FP6), we again delivered more access days to our users than it has been contacted. Due to the limited EC fund BNC itself partly supported the projects in order to provide sufficient beamtime for the high quality projects. All user projects are listed in MS database, but only the part of the delivered access days are claimed.

RID – Technische Universiteit Delft, The Netherlands

Starting in 2006, The Reactor Institute Delft offered transnational access through the NMI3 access program. Even though the Delft reactor is relatively small, its unique polarized neutron facilities as well as its huge capacity for instrumental activation analysis (INAA) have made it possible for users from a other countries to perform research that would otherwise not have been possible.

The INAA technique lends itself to analysis of environmental samples, like air filters, mosses and lichens, and that is the focus that emerges from the corresponding applications.

The allocated beam days for RID appear to be sufficient at this time to offer acces during the first two years of the FP7 program. We do expect to run out of beam days before the FP7 program will end, though.

NPI – Nuclear physics Institute, Rez-Praha, Czech Republic

NPL started a standard user service only with the implementation of I3 infrastructure programs in FP6 and it continues in the similar program within FP7. The Access activity of I3 proved to be essential for profit on both sides - the users and the NPL infrastructure. First of all, it enabled NPL to gain broad experience on the user service from the other facilities all over the Europe, where such programs were already running for a long time. Second, it helped to a substantial part of our users to take advantage of the NPL neutron physics facilities. Users from both old and relatively newly affiliated EU countries and even from the associated states benefit from the Access programme at NPL. The support helps particularly new users to overcome a certain barrier always connected with the use of a new experimental technique. Last but not least, NMI3 has an important financial role for running the NPL neutron physics facilities. Without funding through the beam fee system, any improvements and even smooth running of the user program would be significantly suppressed.

Main scientific areas, in which the NMI3 supported experiments were performed at NPL are engineering, materials science and life sciences.

Description of the publicity concerning the new opportunities for access

ISIS – Science and Technology Facilities Council, Rutherford, UK

A variety of means has been used to publicise the access that has been available under Framework Programme 7 to ISIS:

- a permanent notice on the ISIS Web pages advertising the Access Programme and giving instructions on how to apply (see http://www.isis.stfc.ac.uk/apply-for-beamtime/eu-funding-for-experiments-at-isis9834.html)
- a section for completion in the ISIS electronic proposal submission form;
- advertisements in ‘Neutron News’;
- informal contacts with with EC research teams.

FRM II – Technische Universität München, Germany

The new opportunities are published on the user office’s web page:

http://www.frm2.tum.de/user-office/nmi-3/index.html

In case users have any questions regarding the regulations, there is also a FAQ:

http://www.frm2.tum.de/en/user-office/user-guide/faq/nmi3/index.html

JCNS – Forschungszentrum Jülich, Germany

To inform the scientific audience on the new opportunities for access supported by NMI3 at the instruments of JCNS at FRM II regular e-mails are send out to all users registered in the FRM II user data base (fzj.frm2.tum.de) and members of the international neutron mailing list (www.neutron.anl.gov).

Advertisement for Call for Proposals is published at the international journal Neutron News, within the bi-annual FRM II Newsletter (www.frm2.tum.de/en/aktuelles/info-documents/newsletter/index.html) and at workshops and conferences JCNS participates.

Dedicated information is given within the webpages of JCNS to inform users about access and support (www.jcns.info/jcns_proposals/#) with special information for European users and NMI3 support (www.jcns.info/NMI3/).

SINQ – SμS, Paul Scherrer Institut, Villigen, Switzerland

There are several actions undertaken at SINQ and SμS to publicise the opportunities for access to the facility. A dedicated webpage for the NMI3 access program at SINQ/SμS has been set up: http://www.psi.ch/useroffice/sinqss-nmi3 which summarizes all details about the eligibility within the access programme, the criteria and the modalities for funding as well as the necessary duties for reports. Further general news are published on the dedicated 'SINQ news' page: http://sinq.web.psi.ch/sinq/news.html. Interesting conferences, workshops related to neutron scattering are announced at the online conference calendar: http://www.psi.ch/useroffice/conference-calendar. We also provide regular input to the general 'NMI3 webpage' on the 'Neutron and Muon Web Portal': http://neutron.neutron-eu.net/n_nmi3, whenever important news, deadlines etc. on the access to SINQ/SμS have to be announced. All the webpages listed above are easily accessible since they are directly linked from the webpages of the two facilities and the PSI user office.

Furthermore, two electronic 'calls for proposals' for each facility per year are distributed among the neutron/muon user community by email. In there the option to apply for funding within the NMI3 programme is mentioned explicitly. During the bi-annual PSI Users' meetings, (JUM@P series: http://indico.psi.ch/event/jump11), which are also attended by various potential new user groups, detailed information about the access possibilities and the NMI3 programme is provided, as well.

The PSI Digital User Office, DUO – https://duo.psi.ch - also sends out the notifications and feedback to the proposal authors after the evaluation round and allows the facility management to easily handle the user operation and create statistics. DUO is part of the PSI User Office, which serves as central contact point not only for the neutron and muon users but also for the X-ray synchrotron (SLS) at PSI.

In 2009 PSI launched an electronic newsletter: http://www.psi.ch/info/facility-news. PSI facility news summarizes new options at the PSI user facilities, informs about scientific highlights, calls for proposals, submission deadlines and other interesting news for users. It appears quarterly and is sent out to approximately 10.000 users from the neutron/muon/photon community.

BENSC – Helmholtz Zentrum Berlin, Germany

The HZB web pages are the most important medium for publicising the access opportunities at HZB and informing European researchers about the support they get from the EU through the NMI3 programme. The link to the relevant information is prominently placed at the neutrons web page of the HZB:

https://www.helmholtz-berlin.de/user/neutrons/user-info/eu-access-to-bensc_en.html

A further important measure for informing the neutron community is the "Call for Proposals" sent out twice a year via the neutronsources.org mailing-list which guarantees world-wide dissemination. These efforts are rounded out by continuous advertising in the Neutron News journal and frequent presentations at conferences and workshops.

LLB – Commissariat Energie Atomique, Saclay, France

The opportunities of the ACCESS program at the LLB are detailed in the LLB Web site at the address: http://www-llb.cea.fr/en/Web/hpr_web/HPRWEB0_p.php

- The following items are extensively developed:
- The reactor Orphée
- The Laboratoire Léon Brillouin (LLB)
- The European Community Access Programme to LLB
- Organisation of the User Access Programme
- The LLB-Orphée instruments
- Application forms
- Experimental reports
- Accommodation and logistic support
- Who to contact

A month before the deadline for the submission of the proposals (May 1st and November 1st of each year) a reminder of the call is sent to the mailing list of LLB users and also to the others world-wide neutron facilities and neutron societies. Advertising in the journal “Neutrons News” is also published.

GeNF – GKSS Forschungszentrum Geesthacht, Germany

On our GeNF Web site we have the extensive web page "EU Funding for Experiments at GeNF":

http://www.gkss.de/cms01/central_departments/genf/nmi3/index.html.en

On this page the possibility of NMI3 funding is explained in detail as well as the whole procedure. In the framework of our new research platform "German Engineering Materials Science Centre" (GEMS) we continue this on our new web site:

http://www.gkss.de/cms01/central_departments/gems/use/promotion/index.html.en

In the advertising campaign of our school “Application of Neutrons and Synchrotron Radiation in Engineering Materials Science” we presented the NMI3 funding possibilities Europe-wide. The school which took place between 31.08. and 04.09.2009 in Lauenburg near to Hamburg was funded by NMI3. We communicated the NMI3 funding opportunities to the 51 students with 23 nationalities, coming from 11 different countries of affiliation.

BRR – Magyar Tudomanyos Akademia KFKI, Budapest, Hungary

Several actions have been taken to promote the Access program available at Budapest Neutron Centre under the NMI3-FP7.

BNC website has been dedicated for the access program providing information about the beam time application, deadlines and requirements. This information can also be reached from the European Neutron Portal. BNC also circulates a announcement among the neutron users through internet before each deadline.

The access opportunity to BNC’s facilities is regularly advertised in the Neutron News. BNC also places advertisement in the Progress Report of Budapest Research Reactor which is distributed to the European neutron scientists.

We consider that the most efficient way to reach the European neutron scientists is the personal contact.

International conferences, workshops are utilized for this purpose. BNC organised the 5th Central European School on Neutron Scattering (31 May - 4 June, 2010). We think, that the young attendees (physicists, chemists, biologists) getting acquainted with the neutron techniques and the local circumstances may become our users.

RID – Technische Universiteit Delft, The Netherlands

The opportunities for Access offered at RID are publicized through the institute's website, as well as by handouts offered at appropriate conferences and through the network of scientists working at RID.

NPI – Nuclear physics Institute, Rez-Praha, Czech Republic

NPL facilities opened for external users are listed in database at web page "The Neutron Pathfinder" http://pathfinder.neutron-eu.net/idb, a suitable facility-selection tool for all user accessible neutron instruments in European centres.

The link to the Transnational Access web page http://neutron.ujf.cas.cz/CFANR/access.html of Neutron Physics Laboratory is listed in the Research & Development menu of the home institute (Nuclear Physics Institute of ASCR) web http://www.ujf.cas.cz.

The Transnational Access web page informs the scientific community on the available facilities in the frame of NMI3 Access action, on the research areas investigated using these facilities as well as the on the technical items connected with the experiments at the selected facilities. The proposal submission procedure is listed there as well. The web page also informs on the necessary administrative procedures to be fulfilled before and after obtaining financial support for the experiment within Access activities.

Description of the selection procedure

For list of selection panel members refer to Annex 1 (MS Access Database)

ISIS – Science and Technology Facilities Council, Rutherford, UK

EC researchers wishing to use ISIS apply as part of the normal ISIS procedure for beamtime applications which requires completion of a web-based submission form. There are two calls for experimental proposals in April and October each year; these calls are advertised well in advance.

The ISIS Facility Access Panels meet roughly six weeks after each proposal deadline. They consists of around 70 international experts in the neutron technique and the areas of science to which it is applied (advisers from the Facility are also present, but they do not take part in the experiment selection process). It is also ensured that there are panel members from outside the UK, particularly from European countries. One third of the panel membership is changed each year in order to retire long-serving members and add new ones – details of the present panel composition are given in the database report.

The essential criterion for selection of a proposal by the ISIS Facility Access Panels is its scientific merit. In order to encourage new users and new research groups to use the muon technique, proposals from inexperienced workers are dealt with more favourably. Feedback is always given of the Panels' findings, particularly where a proposal has been rejected or the number of days requested reduced. This feedback is given in the form of a written comment to the applicants.

FRM II – Technische Universität München, Germany

Well-known experts from German and European universities and institutions review and select the proposals only according to their scientific merit. The referees belong to the panel for a period of 3 years on average.

Currently, the selection panel of the FRM II consists of five sub-committees, which review all submitted proposals. Each sub-committee consists of 6 to 8 referees. The five sub-committees are:

- Applied Science I; nuclear and particle physics
- Applied Science II; texture and stress measurements, radiography
- Soft Matter; polymer physics, biophysics
- Magnetism; magnetism, phonons
- Structure; atructure analysis, diffraction

During their meeting they rank and suggest the distribution of the available beam time to the director of the FRM II. The panel meetings are held at Garching twice a year, in March and October.

Shortly after the meeting each main proposer is informed by email, if her/ his proposal was accepted or not. In case it didn't get beam time, an additional email with an explanation for the rejection is sent to the proposer by the secretary of the respective sub-committee.

Priority for the travel reimbursement is given to new users and especially PhD-students. In case the experiment is eligible for the financial support within NMI3, one user per experiment can claim her/ his travel expenses afterwards.

JCNS – Forschungszentrum Jülich, Germany

The governing principle for the selection procedure of JCNS is that of fast evaluation and scientific merit. For this purpose an international review panel has been set in operation. At current the panel consists of 11 European scientists from 6 European countries. At current chair of the panel is Arantxa Arbe of the Center of Material Physics in San Sebastian, Spain. These experts are international well known scientists in their fields with a profound knowledge of neutron scattering to give qualified judgements on the submitted proposals. The area of expertise of the panel members covers polymer and colloid physics, condensed matter physics, chemistry and biology, reflecting the main scientific areas of the submitted proposals.

Experimental proposals are accepted for two deadlines per year. Current next deadline is Oct. 8 2010. To enable a fast evaluation the proposals are refereed by an internet-based procedure. The proposals are distributed by e-mail and through a dedicated and password-secured web site to the referees. For each proposal two reporters are selected by the chairman of the panel. The reporters write short statements on the scientific interest and quality of the proposed work including a suggestion for a rating which are posted on the web site within about two weeks. There all referees can access them and discuss by exchanging e-mails. After about four weeks all panel members send their grades on a scale 0–10 and if necessary a suggestion of reduced experiment time. New users of the facility will be treated preferentially by rating their proposal with a "bonus" on top of the referees' grade. Proposals with an average grade ≤ 4 are immediately rejected. The remaining proposals are accepted in the order of their average grades until the time allocated for the access programme is filled. Exceptions from the order given by the averaged grades from the referees are possible if proposals are not feasible with the instrumentation present at JCNS or single instruments get over- or underloaded in a certain round. Those exceptions have to be approved by the chairman of the panel. Proposals which were not accepted in a certain round due to overload are offered resubmission by the authors with the next deadline.

The final statements of the review panel are sent to the proposers by e-mail in case of final rejection for the current round to give them a guideline to improve their proposal. If a proposal is rejected because of unfeasibility the project manager will explain the reasons.

SINQ – SμS, Paul Scherrer Institut, Villigen, Switzerland

Both SINQ and SμS dispose of international and independent scientific selection panels. The criteria followed to appoint the selection panel members are based on the scientific qualification of the candidates and on the need to cover all fields of research, which are addressed by the proposals received at SINQ/SμS. The panel members are well known experts in the various fields of neutron scattering and muon spectroscopy with an outstanding reputation and publication record. Selection panel meetings at SINQ are organized twice a year at PSI. For SμS one physical meeting of the panel members is organized (winter round) complemented by an electronic evaluation round in the summer. During the reporting period (months 1-18) the following panel meetings took place:

Date	Venue	Panel
Feb 05-06, 2009	PSI	SINQ proposal review committee
June 2009	electronic evaluation	SμS proposal review committee
Jul 02-03, 2009	PSI	SINQ proposal review committee
Jan 27-28, 2010	PSI	SμS proposal review committee
Feb 01-02, 2010	PSI	SINQ proposal review committee
June/July 2010	electronic evaluation	SμS proposal review committee
Jul 01-02, 2010	PSI	SINQ proposal review committee

The composition of the two selection panels, which are also public available on the web:

http://sinq.web.psi.ch/sinq/committee.html & http://lmu.web.psi.ch/research/commit.html

The criteria to select the proposals for funding are in total agreement with the guidelines provided in Annex III to the Grant Agreement, section III-3. Once a proposal is eligible for funding (see Annex III, III-1) the main criterion for selection is its scientific merit classified by the selection panels. Upon equal scientific qualification further criteria are applied such as selection of new user groups or groups from countries without a national neutron/muon source. No further national balancing is applied.

BENSC – Helmholtz Zentrum Berlin, Germany

The HZB operates two large scale facilities, the research reactor BER II and the synchrotron radiation source BESSY II. The beamtime at these facilities is granted in the framework of a peer-reviewed proposal system. To strengthen the synergetic use of neutron and synchrotron radiation, HZB has implemented a common Scientific Selection Panel dealing with proposals for neutron and synchrotron radiation beam time at BER II and BESSY II in joint sessions. For covering the broad scientific spectrum of applications the SSP is subdivided into six scientific colleges, each occupied with typically 10 international experts:

C1 – Soft Matter and Biology

C2 – Macromolecular Crystallography

C3 – Chemistry, Catalysis

C4 – Electronic structures

C5 – Magnetism and Superconductivity

C6 – Material Science and Hard Condensed Matter

There are two proposal rounds per year. The deadlines for submitting the proposals are 1 March and 1 September. The proposals are allocated to the appropriate college as indicated by the proposer. Between 7 to 8 weeks after the deadlines the colleges of the Scientific Selection panel meet at the HZB and discuss and evaluate the proposals in closed parallel sessions. They provide a priority ranking of the proposals based on their scientific merit and give advice on the appropriate amount of beamtime to be granted. Beamtime conflicts between different colleges are discussed and usually settled in a meeting of the college speakers following the college sessions. The final decision is taken by the Scientific Director of the HZB based on the recommendations of the college speakers. The results of the selection process are communicated to the proposers by the user coordinator. Rejected applicants are supplied with a written comment explaining the reasons for the refusal. The dates for the last three sessions of the Scientific Selection Panel were 29-30 April 2009, 6-7 November 2009 and 23-24 April 2010. The meetings took place at HZB Berlin.

LLB – Commissariat Energie Atomique, Saclay, France

To perform an experiment, the researcher must submit a proposal on a special form where he specifies his scientific interest and describes the proposed experiment. Deadlines for submission are: May 1st and November 1st of each year.

Proposals for experiments are selected through a peer review. Selection Committees (SC) are composed by high level scientists from France and European Countries and meet twice a year. The membership of the SC is detailed in the MS Access Database.

The dates and venues of the SC meetings are within this PR1 are the following:

4th and 5th June 2009 / 14th and 15th December 2009 / 14th and 15 June 2010

Experiments to be taken in charge by the ACCESS NMI3 program are selected by the SC on the basis of scientific merit. However, some additional criteria might be taken into account:

- new users
- Countries without neutron facilities.
- experiments involving PhD thesis (or post-docs).

The Selection Committee ranks the proposals in three categories:

A= the proposal is accepted and will be programmed for sure.

B= the proposal will be programmed if additional time is available in the planning of the spectrometers

C= the proposal is rejected because of insufficient scientific quality or because of the overload rate of the spectrometers.

The scientist responsible of the proposal receives an official letter giving the SC grade. When a proposal is graded B our C, an explanation is included in the letter. Sometimes the SC revise the number of beam time claimed in the proposal and then fix a higher or lower number of days allocated.

In 2009, it was found necessary to reorganize and update the structure of the Selection Committees. The old thematic classification was the following:

Theme A: CHEMICAL PHYSICS, BIOLOGICAL SYSTEMS

Theme B: STRUCTURAL STUDIES, PHASE TRANSITIONS

Theme C: MAGNETISM, SUPERCONDUCTIVITY

Theme D: DISORDERED SYSTEMS, MATERIALS

The aim of this reorganization was to make the selection process more efficient because the theme C "Magnetism and Supraconductivity" exceed by double the number of proposals of the other themes. We have merged the subthemes of committees B and C, and we have separated them in 3 committees. The other committees (A and D) remain unchanged. The new thematic classification is the following:

Theme 1: CHEMICAL PHYSICS, BIOLOGICAL SYSTEMS

Theme 2: CRYSTALLOGRAPHIC AND MAGNETIC STRUCTURE

Theme 3: MAGNETISM/ SYNGLE-CRYSTAL SYSTEMS AND THIN LAYERS

Theme 4: DISORDERED SYSTEMS, NANOSTRUCTURED MATERIALS MATERIAL SCIENCE

Theme 5: EXCITATIONS

The list of the sub-themes can be found at the address:
http://www-llb.cea.fr/en/Web/hpr_web/HPRWEB10.php

GeNF – GKSS Forschungszentrum Geesthacht, Germany

All beamline scientists are involved in the internal evaluation process of the technical feasibility of the experiments.

The selection panel of GKSS consists of 36 external and international scientists covering the fields of material science, soft matter research, biology, magnetism and instrument development. Due to the topics of proposals from these reviewers in total 13 were asked for their comments.

The GKSS proposal selection process is very different from other facilities. We encourage our users to **continuously submit proposals** which are forwarded to the reviewers (usually two persons per proposal) by email directly after reception and proof of technical feasibility. In general the reviewers are asked to reply within two weeks on a report form on which they should state the quality of the proposal (by ranking and text explanation, see GeNF Review Form in Annex I) and comment on the amount of beamtime applied for. If the reviewers disagree by more than one rank a third reviewer is included. If the proposal is approved the beamline scientist organizes fast access to the facility. We are aiming at giving beamtime within 3 months after application, i.e. faster than at most other facilities. In order to fulfil this service a serious discussion of the proposal between applicants and beamline scientists **before** submission of the proposal takes place. This is the reason why in general the quality of the proposals is high and therefore the rejection rate comparatively low. This feedback procedure leads to 'just in time' applications because the users rely on our capability to give them fast access after acceptance of their proposal.

If even after thorough discussion previous to submission a proposal is rejected, the authors are notified by sending the anonymous reviewer's comments. Explanations are given by our experts if the users still have questions about the rejection. They are encouraged to resubmit an improved proposal if the reasons for rejection only have been missing information or an unclear description of the experiment.

All these efforts are necessary because a significant amount of users are completely unskilled with neutron experiments. To help them use our facilities is one of our specialities.

BRR – Magyar Tudomanyos Akademia KFKI, Budapest, Hungary

BNC established two deadlines (May 15, October 15) for proposal submission to ensure the high level scientific evaluation and schedule the available beam time. Next to the regular selection process fast track application is also possible in especially important cases. The selection and decision is made via internet at the spring cycle and on the annual meeting in autumn.

The *principals* of the selection process:

- All distributed proposals shall meet BNC's format and content requirements.
- The same evaluation procedure is applied in case of all proposals to ensure consistency.
- All experimental proposals is reviewed and evaluated by the panel members responsible for the specific scientific field.
- No interested party is involved in the selection process.
- The progress of the decision-making process can be followed through internet.

The User Selection panel bases its selection on scientific excellence and gives priorities to

users who have not previously used the infrastructure,

users who are working in countries where no such research infrastructure exits.

Feedback is given to the applicants particularly where the number of requested days reduced or the proposal has been rejected. In case of rejected proposal the instrument responsible contacts the applicant and assists him/her to improve the proposal.

The members of the User Selection Panel are experienced scientists understanding the technical details of the proposed work programs and the capabilities of BNC's instruments. The composition of the panel is international; from the 11 members 2 members are representing Hungarian institutions, 9 members are from the leading European neutron centres (ILL, LLB, PSI) or universities. The competence of the panel covers the entire research area expected by the neutron proposals.

RID – Technische Universiteit Delft, The Netherlands

At RID, proposals are sent to appropriate, preferrably independent reviewers as they come in. Because of the small number of proposals and the wide variety of subject matter at stake, this is the only feasible way for the institute. The list of panel members may therefore grow throughout the program. The reviewers are asked to judge the scientific quality, feasibility and justifiability for European funding. If proposals are rejected, the applicant is informed by email. The applicant then also receives the reviewer's comments.

There are no selection panel meetings for RID.

NPI – Nuclear physics Institute, Rez-Praha, Czech Republic

All the proposals are peer reviewed by the NPL international Selection Panel. The main criterion for acceptance is scientific excellence of the project followed by the intention to fund young scientists, new neutron users and also projects from countries without a national neutron source.

Before passing the proposals to the members of the Selection Panel, their technical feasibility is considered by the instrument responsible of the particular facility. It can result in a request to modify the proposal according to the available equipment or can also cause a postponement of the proposal due to the fabrication of the necessary equipment.

The NPL Selection Panel bases its selection on scientific merit. The proposal is thus accepted/rejected following these criteria:

1) scientific excellence (given by the assessment by the Selection Panel),
2) available beam time,
3) available financial sources for the support

The main proposer is informed about the general acceptance/rejection of the proposal and about the success of their application for funding.

The author of the rejected proposal is notified, the reason for the rejection is clearly stated and the further actions to be taken are suggested (e.g. further discussion with the instrument responsible on the feasibility, referee's suggestions to improve proposal).

The members of the User Selection Panel were selected on the basis their

1) knowledge on neutron scattering,

2) their specialization in one or more fields covered by the facilities included in the programme.

There are no ordinary meetings of the User Selection Panel. The correspondence is carried out electronically which brings about temporal flexibility to the selection procedure. Every set of proposals is sent to all the members of the User Selection Panel. One of the members of the Panel, who is a top expert in the related field is asked to provide a written report on the given proposal. The other members of the panel can comment on the proposal as well.

Transnational Access Activity

For comparison of the 11 facilities, refer below to the Table 1 and **Table 2**

For list of user projects refer to Annex 2 (MS Access Database)

For list of users refer to Annex 3 (MS Access Database)

Table 1: ***Beam days [d] per facility with regards to different thematic fields***

Scientific Field (months1-18)	ISIS Neutron	ISIS Muon	FRM II	JCNS	SINQ Neutron	SμS Muon	BENSC	LLB	GeNF	BRR	RID	NPI
Chemistry	15	2	51	12	20	2	51	62	43	10	0	0
Engineering & Technology	6		78	4	2	2	60	8,5	17	2	0	36
Earth Sciences & Environment	1		36	12	23	0	0	7	0	6	22	0
Energy	2	1	24	0	5	0	0	17	0	0	0	0
Humanities	0		23	0	6	0	36	7,5	0	20	5	0
I & C Technologies	2	2	6	0	11	0	0	23	0	0	0	0
Life Sciences & Biotech (Health)	10		8	50	30	0	56	43,5	22	5	5	23
Material Sciences	12	1	72	21	111	16	98	30,5	22	34	10	18
Physics	23	3	223	60	226	164	329	58	7	78	7	0
Total	**69**	**9**	**521**	**159**	**434**	**184**	**630**	**257**	**111**	**155**	**49**	**77**
% fields non-physics	**67%**	**67%**	**57%**	**62%**	**48%**	**11%**	**48%**	**77%**	**93%**	**50%**	**86%**	**100%**

Table 2: ***Transnational Access Activity of the 10 facilities***

The figures reported below vary from the figures in the Form C (financial report) as they reflect the real effort of the facilities to support EU users, beyond the EC support.

Organisation short name	*Short name of infrastructure*	*estimated total cost* [14]	*Unit of access*	*Estimated number of users*	*Estimated number of projects*	*PR1 reported users*	*PR1 reported Beam days*	*T&S cost spent (€)*	*beam fee spent (€)*	*Publication FP7*	*including NMI3 FP6 project**	*Publications to come for experiments of this period*
STFC	ISIS-Neutrons	211,254,000	53	103	41	69	47	24,400	494,299	3		
STFC	ISIS-Muons	211,254,000	11	30	9	24	11	5,081	133,047	3		
TUM	FRM II	141,141,187	160	52	34	100	521	76,053	1,719,300	3	5	
FZJ	JCNS	37,415,418	102	69	17	27	159	36,560	524700	2	2	
PSI	SINQ	36,952,893	223	83	41	102	434	62,000	1,041,600	4	20	
PSI	SμS	12,768,838	105	41	34	49	184	25,500	441,600	4	16	
HZB	BENSC	72,186,896	240	110	55	173	630	105,000	1,573,866	3	28	
CEA	LLB	79,352,940	200	62	38	68	257	65,656	861,706	10	20	
GKSS	GeNF	60,773,272	62	25	16	24	111	17,746	353,102	14		
BNC-AEKI	BRR	17,821,920	100	48	21	25	155	13,537	229,400	3	9	
TUD	RID	8,963,153	90	10	18	11	49.2	3,200	68,880	0		8
NPI	NPI	5,134,209	68	14	8	12	77	5,159	92,400	2	7	3

Grey cells are direct costs (T&S cost do not include overheads)

* Publications: between Jan 09 – Jul 10 based on experiments funded by NMI3/FP7

Publications including FP6: publications published between Jan 09 – Jul 10 based on experiments funded by all NMI3 projects incl. FP6

[14] ***Estimated total costs of providing total quantity of access to the installation over the duration of the project (€)***

Scientific Output of the users at the facilities

ISIS highlights

Many of the experiments performed under the current Access programme have been run within the past 6 months. Therefore publications are in preparation and have not yet appeared.

One significant highlight, however, has been the Access-funded work of VO de Haan et al. Their work, exploring a fundamental effect in the way that neutrons reflect from surfaces, is notable for a number of reasons:

- It was the first publication from ISIS Second Target Station
- The data were taken using the neutron polarisation capabilities off the OffSpec reflectometer, developed collaboratively between ISIS and TU Delft.
- It was the first direct, absolute, experimental determination of the Goos-Hänchen shift for a particle experiencing a potential well as required by quantum mechanics: namely, wave-particle duality – and was published in Physical Review Letters.
- The story has been reported in Physics World and Materials World, in addition to the original publication in Physical Review Letters.

A brief summary is given here.

Observation of the Goos-Hänchen Shift with Neutrons

Victor-O. de Haan, Jeroen Plomp, Theo M. Rekveldt, Wicher H. Kraan, and Ad A. van Well (Delft), Robert M. Dalgliesh and Sean Langridge (ISIS)

Phys. Rev. Lett. 104, 010401 (2010)

ISIS RB No.: RB920144

Instrument: OffSpec

Abstract from **Phys. Rev. Lett. 104, 010401 (2010)**

The Goos-Hänchen effect is a spatial shift along an interface resulting from an interference effect that occurs for total internal reflection. This phenomenon was suggested by Sir Isaac Newton, but it was not until 1947 that the effect was experimentally observed by Goos and Hänchen. We provide the first direct, absolute, experimental determination of the Goos-Hänchen shift for a particle experiencing a potential well as required by quantum mechanics: namely, wave-particle duality. Here, the particle is a spin-polarized neutron reflecting from a film of magnetized material. We detect the effect through a subtle change in polarization of the neutron. Here, we demonstrate, through experiment and theory, that neutrons do exhibit the Goos-Hänchen effect and postulate that the associated time shift should also be observable.

General summary

The OffSpec reflectometer on the new ISIS Second Target Station has been used to finally make the connection between the reflection of particles and waves as required by quantum mechanics. The phenomenon is a long established theory, but has not until now been seen. Whilst the discovery currently lies in the realm of pure physics, these results may initiate new developments in electronics, complementing the wave equivalent already used for photonics and metrology.

A team led by Victor de Haan from the Delft University of Technology (Netherlands) and ISIS scientists Rob Dalgliesh and Sean Langridge has proved experimentally for the first time that particles (in this case, neutrons) slide along a surface before they are reflected. This means that particles are reflected from a different point to the one where they arrived.

The spatial shift of a reflection was first suggested by Isaac Newton in the 17th century. Later in 1947 Goos and Hänchen used light to provide experimental evidence of Newton's suspicions and so was born the "Goos-Hänchen shift". The recent discovery from work at ISIS not only supports the ideas and work of Newton, Goos and Hänchen, but also proves that when particles are reflected they behave in exactly the same way as light, as predicted from quantum theory.

"Our results show that particles, in this case neutrons, behave in exactly the same way as light when they are reflected," says Professor Sean Langridge, an STFC research fellow at ISIS. "The capabilities of the new Offspec instrument that we have built at the ISIS second target station have allowed us to see this at the quantum level for the first time. The results provide us with further experimental evidence of the correctness and beauty of quantum mechanics and that ideas ranging from Newton to our present understanding of quantum phenomena are well founded," he said.

The experiment took place at the new second target station at the ISIS on the Offspec neutron instrument. The result was achieved by shining a beam of polarised neutrons onto a film of magnetic material and observing the minuscule change in polarisation after reflection. This incredible sensitivity was only possible through the development of the Offspec instrument, a collaboration between ISIS and the Delft University of Technology.

"This unique instrument as well as the first publication is the result of outstanding cooperation between the ISIS team and researchers from the Reactor Institute at Delft," said Professor Tim van de Hagen, Director of the Reactor Institute Delft

RB920144

Observation of the Goos-Hähnchen Shift with Neutrons

Victor-O. de Haan, Jeroen Plomp, Theo M. Rekveldt, Wicher H. Kraan, and Ad A. van Well, Robert M. Dalgliesh, Sean Langridge,

Phys Rev Lett 104 (2010) 010401

RB920144

Coherence approach in neutron, x-ray, and neutron spin-echo reflectometry

Victor O. de Haan, Jeroen Plomp, M. Theo Rekveldt, Ad A. van Well, Robert M. Dalgliesh, Sean Langridge, Amarante J. Böttger and Ruud Hendrikx

Phys Rev B **81** (2010) 094112

RB920181

Octahedral tilting in Pb-based relaxor ferroelectrics at high pressure

Bernd J. Maier, Ross J. Angel, William G. Marshall, Boriana, Mihailova, Carsten Paulmann, Jens M. Engel, Marin Gospodinov, Anna-Maria Welsch, Dimitrina Petrovae, and Ulrich Bismayera

Acta Cryst. B66 (2010) 280–291

FRMII highlights

The wide range of applications concerning the use of neutron scattering is reflected in the publications so far appeared from the first 18 months of user operation in the NMI3 consortium at the FRM II. They range from fundament research in solid state physics, life science to engineering research. The examples show results from experienced groups like the institute from Günther Redhammer, Switzerland to completely new users as Pérez-Landazábal et al.(Spain) investigating the lattice dynamics of ferro-magnetic shape memory alloys. Quite numerous are the applications and respective successful experiments from university groups of the UK in the field of engineering science investigating joint from ordinary welding to very modern friction steer welding.

Title: *Magnetic and nuclear structure and thermal expansion of orthorhombic and monoclinic polymorphs of CoGeO3 pyroxene*

Main author: *Günther Josef Redhammeret al.*

Title of periodical or series: *Physics and Chemistry of Minerals*

Number, date or frequency: *37 (2010)*

Relevant pages: *311-332*

Permanent identifiers http://dx.doi.org/10.1007/s00269-009-0335-x

User Project: FRM-II_3099

Title: *From Powder to Solution: Hydration Dependence of Human Hemoglobin Dynamics Correlated to Body Temperature*

Main author. *Andreas Stadler et al.*

Titel of periodical or series: *Biophysical Journal*

Number, Date: *96/12 (2009)*

Relevant pages: *5073-5081*

Permant identifiers: http://dx.doi.org/10.1016/j.bpj.2009.03.043

User Project: FRM-II_2898

Title: *Determination of new K_0 values for prompt gamma activation analysis at Budapest*

Main author. *Zsolt Revay et al. .*

Titel of periodical or series: *Nuclear Instruments and Methods in Physics Research A*

Number, Date: *2010*

Relevant pages: *in press*

Permant identifiers: http://dx.doi.org/10.1016/j.nima.2009.12.068

User Project: FRM-II_2903; FRM-II_3586

Title: *Investigations of stone consolidants by neutron imaging.*

Main author. *F. Hameed et al.*

Titel of periodical or series: *Nuclear Instruments and Methods in Physics Research A*

Number, Date: *605 (2009)*

Relevant pages: *150-153*

Permant identifiers: http://dx.doi.org/10.1016/j.nima.2009.01.139

User Project: FRM-II_398

Title: *Lattice dynamics and external magnetic-field effects in Ni-Fe-Ga alloys*
Main author. *J.I. Pérez-Landazábal et al.*
Titel of periodical or series: *Physical Review B*
Number, Date: *80 (2009)*
Relevant pages: *144301*
Permant identifiers: http://dx.doi.org/10.1103/PhysRevB.80.144301
User Project: FRM-II_1314

Title: *Two-Dimensional square-lattice S=1/2 antiferromagnet* $Cu(pz)_2(ClO_4)_2$
Main author. *N. Tsyrulin et al.*
Titel of periodical or series: *Physical Review B*
Number, Date: *81 (2010)*
Relevant pages: *134409*
Permant identifiers: http://dx.doi.org/10.1103/PhysRevB.81.134409
User Project: FRM-II_302; 521

Title: *Quantum Effects in a Weakly Frustrated S=1/2 Two-Dimensional Heisenberg Antiferromagnet in an Applied magnetic Field*
Main author: *N. Tsyrulin et al.*
Titel of periodical or series: *Physical Review Letters*
Number, Date: *102 (2009)*
Relevant pages: *197201*
Permant identifiers: http://dx.doi.org/10.1103/PhysRevLett.102.197201
User Project: FRM-II_302; 521

Title: *Measured residual stress distributions for low and high heat input single weld beads deposited on to SA508 steel*
Main author: *J.A. Francis et al.*
Titel of periodical or series: *Materials Science and Technology*
Number, Date: *25(3) (2009)*
Relevant pages: *325*
Permant identifiers: http://dx.doi.org/10.1179/174328408X372074
User Project: FRM-II_544; 964

JCNS highlights

During recent beam time at NMI3 supported European users at instruments of JCNS certain scientific important projects in the area of environmental sciences, life sciences, physics and material sciences could be performed.

The group of F. Juranyi et al of PSI, Switzerland (JCNS-2584), investigated the water diffusion in clay systems, considered as possible storage environment for radioactive waste repositories. Here diffusion coefficients of water at super-cooled temperatures were investigated to prove correct values to calculate the migration of water in clay minerals, which is important for possible storage times of waste material in this environment.

Self-assembling of small molecules to form larger aggregates and complex structures is a key process in the organisation of living systems on the molecular level. The aggregation of short peptide strands to form fibres and three-dimensional networks was investigated by small angle neutron scattering by the group of A. Saiani of the University of Manchester, UK (JCNS-2637). They were able to investigate the influence of the hydrophobicity of the peptides on the aggregation behaviour leading to a better understanding of the governing processes of peptide aggregation in living organisms and their influence on the mechanical properties of cells (A. Saiani et al., Soft Matter, 5, 2009, 193-202).

A new class of antio-cancer drugs based on ruthenium complexes have been studied by small angle neutron scattering by the group of L. Paduano et al of the University of Naples, Italy (JCNS-3373, JCNS-3923). Size and shape of the nanovectors were investigated which are now prepared to be used in in-vitro tests to check the anti-tumoral characteristics of the aggregates (M. Vaccaro et al., Soft Matter, 5, 2009, 2504-2512).

The dynamical coupling of water and folded and unfolded proteins to understand the mechanism and dynamic of protein folding was studied by M. Weik et al of IBS, France (JCNS-2698, JCNS-3346, JCNS-3949), using elastic and quasi-elastic neutron scattering. Differences in the hydration-water motions between folded and unfolded proteins were found which will help to understand the function and dynamics of unfolded proteins in life processes.

Hydrogen embrittlement of ultra high strength steel is a major limitation for lowering car weight and gas emission. M. Benoit et al. of the University Grenoble (JCNS-3318), France have used small angle neutron scattering to study the role of precipitates in hydrogen trapping in steel. Preliminary results show possible temperature dependent trapping of hydrogen by the precipitates and may help to develop stable precipitates to entrap hydrogen permanently.

JCNS-1639:

Neutron scattering study of the dynamics of a polymer melt under nanoscopic confinement

M. Krutyeva et al.

J. Phys. Chem.; 131; American Institute of Physics; 2009; 174901-1-174901-11

JCNS-1255:

Colloidal particles composed of amphiphilic molecules binding gadolinium complexes and peptides as tumor-specific contrast agents in MRI: physico-chemical characterization

M. Vaccaro et al.

Soft Matter; 5; The Royal Society of Chemistry; 2009; 2504-2512

JCNS-2637:

Self-assembly and gelation properties of α-helix versus β-sheet forming peptides

A. Saiani et al.

Soft Matter ; 5; The Royal Society of Chemistry; 2009; 193-202

JCNS-2656:

Self-assembled nanoparticles from a block polyelectrolyte in aqueous media: structural characterization by SANS

A. Papagiannopoulos et al.

J. Phys. Chem. B; 114; American Chemical Society; 2010; 7482-7488

SINQ & SμS highlights

Two of the highlights mentioned below (Carminati et al and Maeter et al) have been selected for a highlight presentation during the recent NMI3 General Assembly in Barcelona (May 10-12, 2010).

proposal Nr: SINQ_20090505

main proposer: M. Pregelj, Slovenia, email: matej.pregelj@ijs.si

Title: Low- and High-Temperature Magnetic Structure of Novel Multiferroic FeTe2O5Br System

Topic: Information Technologies, Materials Sciences, Condensed Matter Physics

Abstract: *Magnetic structure of novel multiferroic $FeTe_2O_5Br$ system was studied by single crystal neutron diffraction in low- and high-temperature regimes. Detailed investigation revealed that in the high-temperature phase, between T_{N1}=11.10(5) K and T_{N2}=10.75(5) K, magnetic moments are almost parallel to the b axis (φ=-75(5)°) and their orientation is almost temperature independent, while below T_{N2} magnetic moments turn with decreasing temperature until at ~10.2 K they reach φ=-45(5)°. No changes in the low-temperature phase have been found down to 60 mK.*

proposal Nr: SINQ_20081333

main proposer: M. Boehm, Grenoble, email: boehm@ill.fr

Title: Determination of the Magnetic Structure of CuCrS2 by Spherical Neutron Polarimetry

Topic: Materials Sciences, Condensed Matter Physics

Abstract: *$CuCrS_2$ is a triangular lattice Heisenberg antiferromagnet with a rhombohedral crystal structure. Neutron diffraction results revealed a magnetoelastic phase transition at T_N = 37.5 K which comprises a lattice distortion and a long-range order of magnetic moments. The propagation vector describes an incommensurate magnetic state with $\mathbf{k}_{mag}$ = (-0.493,-0.087,1.25). Two possible orientations of magnetic moments have been identified by the refinement of neutron powder diffraction pattern. Therefore, the aim of this proposal was to use spherical neutron polarimetry for the discrimination of both possible solutions.*

proposal Nr: SINQ_20081291

main proposer: S. Prevost, Berlin, email: prevost.sylvain@gmail.com

Title: Deformation of surfactant assemblies in a magnetic Room Temperature Ionic Liquid under magnetic field

Topic: Earth and Environment

Abstract: *The present experiment focuses on the possible deformation of self-assembled aggregates in a magnetic room- temperature ionic liquid (MRTIL) under magnetic field. With a 1.2 Tesla field, only a small effect is seen. This opens the door to new experiments under larger fields, yet calls for the optimization of the ternary microemulsions used to amplify the changes observed.*

proposal Nr: SINQ_20081342

main proposer: A. Carminati, Leipzig, email: andrea.carminati@ufz.de

Title: On the way to roots: The journey of water across the soil-plant system

Topic: Life Sciences

Abstract: *How does water enter the roots? Existing models of root water-uptake predict a decrease of water towards the roots, with water moving from wetter (far a way from the root surface) to dryer (adjacent to root surface) regions. But neutron radiography showed the opposite: during a drying period the soil close to roots ap- peared wetter than the bulk soil. Interestingly, the picture reversed after irrigation. Such observations are explained by mucilage exuded by roots. Mucilage favors water availability to plants during drying but on the other hand it decreases the water storage in the root zone after irrigation. The observed dynamics have po- tential applications for improving water-use efficiency and crop production.*

proposal Nr: SµS_20081386

main proposer: T. Lancaster, Oxford, email: t.lancaster1@physics.ox.ac.uk

Title: Molecular Magnetism

Topic: Materials Sciences, Condensed Matter Physics, Information Technologies

Abstract: *In two-dimensional (2D) systems, muon-spin relaxation has been shown to be able to detect transitions to long range magnetic order that are almost invisible to more conventional techniques. We highlight results from our recent SµS experiments on a new compound based on a highly 2D molecular magnetic paradigm and investigations into role of the exchange anisotropy in fostering magnetic order.*

proposal Nr: SµS_20090654

main proposer: H. Maeter, Dresden, email: h.maeter@physik.tu-dresden.de

Title: Magnetic and superconducting properties of iron pnictides with perovskite oxide layers

Topic: Materials Sciences, Condensed Matter Physics, Energy

Abstract: *As in the cuprates, an enhanced structural two-dimensionality increases the superconducting transition temperature of Fe-based superconducturs. Hence, great experimental and theoretical effort has been devoted to the search of new Fe-based superconductors with larger inter-planar distance. In 2009, we investigated three compounds of the newly discovered (M_2Pn_2)($A_4M_2O_6$) system in which the Fe-pnictide layers are separated by perovskite oxide layers with the largest inter-planar distance of ~1.6 nm for Fe-based superconductors known up to now. Here, we report on their magnetic and superconducting properties as determined by zero and transverse field* µ*SR.*

BENSC highlights

Material Science:

HZB-Neutrons_NMI3_II-1505, Instrument E3

M. Schöbel[1], L. Weber[2], P. Dobron[3], R. Wimpory[4], H.P. Degischer[1]

Institute for Materials Science and Technology, TU Vienna, Austria[1]

Laboratory for Mechanical Metallurgy, EPF Lausanne, Switzerland[2]

Department of Metal Physics, Charles University Prague, Czech Republic[3]

Helmholz Zentrum Berlin, Wannsee, Germany[4]

Understanding stress induced delamination and its consequences in diamond reinforced aluminium composites for heat sink applications

In power electronic devices like IGBT (Insulated Gate Bipolar Transistors) baseplate materials are needed, which combine high thermal conductivity (TC) with low thermal expansion (CTE). High heat flux through the baseplate into the heat sink is needed for cooling, and the low CTE reduces delamination between the baseplate and the ceramic chips during operation. Commonly, SiC particle reinforced Aluminum (Al-SiC) is used combining the thermal properties of metal (matrix) with ceramics (reinforcement). To increase the performance of such systems composites with higher thermal conductivity have to be developed. Al-CD (Aluminum-Carbon Diamond) composites are promising, as they use the best known thermal conductivity of Diamond particles embedded in an Aluminum matrix. The low reactivity and wettability of Diamonds with a matrix metal during infiltration makes demands on production. High micro stresses during changing temperature (CTE mismatch) can be expected which lead to delamination at the interfaces. Strong bonding is needed to increase long term stability of the composite under service conditions.

In situ neutron diffraction was made to investigate load transfer from the matrix into the particles during tensile tests and thermal cycling. Neutron radiation was chosen due to the high penetration depth, which is important for in situ scans in the bulk material and the big gauge volumes, implementing enough diamond single crystals (Ø ~ 100 / 50 µm) for good grain statistics. The micro stresses could be compared to correlated acoustic emission measurements and high resolution synchrotron tomography to understand stress induced delamination and its consequences.

Cultural Heritage:

HZB-Neutrons_NMI3_II-1551, Instrument V7

[1]R. Triolo, [2]N. Kardjilov, [2]F. Wieder, [3]I. Ruffo, [1]G. Giambona, [1]V. Benfante

[1]Universita di Palermo, Italy

[2]Helmholtz-Zentrum Berlin, Germany

[3]ITC „L. Sturzo", Bagheria, Italy

Identifying ancient trade routes

The Mediterranean Sea was an important route that allowed for trade and cultural exchange between emergent peoples of the region of Mesopotamian, Egyptian, Phoenician, Carthaginian, Greek or Roman culture, just to mention a few of them. Therefore, it is not surprising that along the commercial routes of the Mediterranean Sea there has been a heavy traffic of ships carrying lead materials, and especially ingots many used as ballast. Occasionally some of the ships sank and their load was buried in sea water for centuries. Clearly, a careful analysis of the lead ingots recovered from sunken ships will add information of archaeological interest. In fact, all the ingots show rectangular areas carrying stamped marks which are a combination of characters and images. In a sense these marks represent a sort of trademark of great importance for archaeologists, as possibility of reading the characters and seeing the images would allow one to determine with high accuracy the age and the producer of the find and a systematic mapping of the finds would make it possible to identify ancient trade routes.

The area containing the marks, however, is completely covered with corrosion products, salt deposits and algae, so it would be necessary to scrape the surface layers to reach the stamped region, an invasive operation which one would like to avoid. Experiments performed at the instrument V7 of the HZB clearly demonstrated that the trade marks can be made visible by neutron tomography without prior manipulation of the ingots. This represents an important progress in cultural heritage studies.

Life Science:

HZB-Neutrons_NMI3_II-1505, Instrument V1

J. Preu[1], Th. Hauss[2], Th. Gutberlet[3]

[1]Niels Bohr Institute,Copenhagen, Denmark

[2]Helmholtz Zentrum Berlin, Germany

[3]Forschungszentrum Jülich, Germany

The interaction of Angiotensin II with model membranes studied by neutron diffraction

Cardiovascular diseases are a growing problem in particular in the Western World. Stroke, heart attacks,heart failure and arterial aneurysms are often a result of persist hypertension. In less than 10 % of the cases the elevated blood pressure can be related to a medical cause, like kidney diseases or tumors. In the majority of the cases a dysfunction in the renin-angiotensin system (RAS) is occuring. The RAS plays a critical role in circulatory homeostasis. Part of this system is the peptide hormone Angiotensin II (Ang II), a potent vasoconstrictor that aids in the blood pressure regulation, as well as in body-fluid balance maintenance. The octapeptide Ang II derives from the precursor from the liver and is acting on the heart, in both endocrine and paracrine fashion. It regulates contractility, remodelling, growth, apoptosis, and reduces cell coupling and conduction velocity in cardiac muscles. Ang II has two major receptor subtypes, the Ang II type 1 receptor (AT1 receptor) and the Ang II type 2 receptor (AT2 receptor). In addition Ang II acts on the membrane. It is of great importance to understand the interaction of Ang II and the membrane in detail. Neutron diffraction provides a unique possibility to study this interaction.

For the experiments the peptide Ang II was dissolved in buffer and chain-deuterated DMPC as model-membrane former added. The dispersion was then deposited on a quartz wafer and dried. By this procedure ordered bilayer stacks of chain-deuterated DMPC were formed. Diffraction peaks up to the 5th order could be measured on the diffractometer V1. These experiments allowed the determination of the position of the peptide in the membrane with a high special resolution. It was found that the peptide is accumulating close to the lipid head groups and not penetrating into the hydrophobic region of the bilayer. This is also in accordance with previous small angle neutron scattering measurements.

LLB highlights

Field	Title of the proposal	authors	Aim of the proposal Why a highlight ?	Applications
Information and Communication technologies	Understanding the mechanism of spin delocalization in the 3D antiferromagnet Rb2FeCl5:H2O	Javier CAMPO and Clara RODRIGUEZ BLANCO (PhD studient). Spain	- Single molecular magnets, (SMMs) represent the smallest possible magnetic devices and are a controllable, bottom-up approach to nanoscale magnetism. - The studies of spin density distribution is a neutron technique very specific to our facility. Only 2 spectrometers available in the word, 1 at the ILL and another at the LLB. - Spanish users, no national facility. -	Potential applications of SMMs include quantum computing, high-density information storage and magnetic refrigeration
Health	Interaction of 1-Alkanols with lipid bilayers from monosaturated phosphatidycholines	Balgavy PAVOL and Daniela UHRIKOVA	- Study of the molecular mechanism of ion channel function inhibition induced by iintercalation anasthetics into membrames. - “human health” is a topic with great social impact - Slovak users, no national facility -	Understanding anaestesia
Health	Formation of diblock copolymer micelles in partially miscible solvents	Petr KADLEC and Petr STEPANEK	- Fundamental studies of the formation of diblock copolymer micelles. - Important number of high level publications - “human health” is a topic with great social impact	application s in drug design and delivery (pharmacology)
Cultural Heritage	Oil droplets embedded in a permanent hydrogel matrix for conservation of Cultural Heritage	Debora BERTI and Piero BAGLIONI	- structural characterization of a microemulsion cosolvents), which can be embedded into a chemical gel formed by the crosslinking of a PEG with an acrylamide derivative. - Support of Cultural Heritage conservation programs - Italian users, no national facility	The motivation is the application of these complex fluids to the removal of resins from frescoes and canvases (“reintelage”). Insight into the resin removal mechanism.

LLB: Following publications are resulting out of the former **FP6** project:

NAME N° PROJECT	LABORATORY	TITLE	REVIEW	AUTHORS
HINKOV Vladimir FP6	Max-Planck-Institute for Solid-State Research, Germany	Strengh of the spin-fluctuation-mediated pairing interaction in a high-temperature conductor	**NATURE PHYSICS n°1180 18 jan 2009**	T. Dahm, V. Hinkov, S. V. Borisenko, A. A. Kordyuk, V. B. Zabolotnyy, J. Fink, B. Büchner,,,,
FIORI Fabrizio FP6	Università Politecnica delle Marche - Dip. SAIFET, Sez. di Scienze Fisiche,CNISM - MATEC, Laboratorio Regionale delle Marche Via Brecce Bianche, 60131 Ancona,Italy	Small-Angle Neutron Scattering characterization of Al2O3/Ni–P nanocomposites	**Materials Science and Engineering B 152 (2008) 136–139**	F. Fiori , E. Girardin, G. Albertini , K. Konopka, F. Rustichelli
BAGLIONI Piero FP6	Univ Florence, Dept Chem, I-50121 Florence, Italy	Small-angle neutron scattering of percolative perfluoropolyether water-in-oil microemulsions	**J. Phys. Chem. B, 114, 3855 (2010)**	M. Laurati, C. M. C. Gambi, R. Giordano, P. Baglioni, J. Teixeira
MERGIA Konstantina FP6		Oxidation behaviour of SiC coatings,	**Applied Physics A 92 (2008) 387-395**	K. Mergia, D. Lafatzis, N. Moutis, Th. Speliotis, G. Apostolopoulos and F. Cousin
UHRIKOVA Daniela FP6	fpharm.uniba.sk	Structural changes in dipalmitoylphosphatidylcholine bilayer promoted by Ca2+ ions: a small-angle neutron scattering study,	**Chem. Phys. Lipids 155, 80-89 (2008)**	UHRÍKOVÁ D., KUČERKA N., TEIXEIRA J., GORDELIY V.I., BALGAVÝ P.
UHRIKOVA Daniela FP6	fpharm.uniba.sk	Hydrophobic thickness, lipid surface area and polar region hydration in monounsaturated diacylphosphatidylcholine bilayers: SANS study of effects of cholesterol and beta-sitosterol in unilamellar liposomes,	**Biochim. Biophys. Acta 1778, 2627-2632 (2008)**	GALLOVÁ J., UHRÍKOVÁ D., KUČERKA N., TEIXEIRA J., BALGAVÝ P
JOVARI PAL FP6		Topological and chemical short range ordering in Co43Fe20Ta5.5B31.5 metallic glass,	**Phys. Rev. B 79 212201 (2009)**	I. Kaban, P. Jóvári, M. Stoica, J. Eckert, W. Hoyer, B. Beuneu
JOVARI PAL FP6		Short range order of Cu-Zr metallic glasses,,	**J. Alloys and Compounds 485 163 (2009**	N. Mattern, P. Jóvári, I. Kaban, S. Gruner, A. Elsner, V. Kokotin, H. Franz, B. Beuneu, J. Eckert,
JOVARI PAL FP6		Atomic structure of As2S3-Ag chalcogenide glasses,,	**J. Phys.: Condens. Matter 21 395801 (2009)**	I. Kaban, P. Jóvári, T. Wagner, M. Frumar, S. Stehlik, M. Bartos, W. Hoyer, B. Beuneu, M.A: Webb,
JOVARI PAL FP6		The structure of As3Se5Te2 infrared optical glass, J. Alloys and Compounds 488 39 (2009),	**J. Alloys and Compounds 488 39 (2009)**	P. Jóvári, B. Bureau, I. Kaban, V. Nazabal, B.Beuneu, U. Rütt

LLB: Following publications are resulting out of the present **FP7** project:

NAME N°PROJECT	LABORATORY	TITLE	REVIEW	AUTHORS
CABRAL Joao FP7 9971	Dr. João T. Cabral Department of Chemical Engineering, ACE 516 Imperial College London London SW7 2AZ, UK	Small Angle Neutron Scattering from the Highly Interacting Polymer Mixture TMPC/PSd: No Evidence of Spatially Dependent χ Parameter	**MACROMOLECULES Volume: 42 Issue: 24 Pages: 9528-9536 Published: DEC 22 2009**	Cabral JT, Higgins JS
HINKOV Vladimir FP7 9509	Max-Planck-Institute for Solid-State Research, Germany	Normal-state spin dynamics and temperature-dependent spin-resonance energy in optimally doped BaFe1:85Co0:15As2	**NATURE PHYSICS n°1483 20 MAR 2010**	D. S. Inosov, J. T. Park1, P. Bourges, D. L. Sun, Y. Sidis A. Schneidewind, K. Hradil, D. Haug,C. T. Lin, B. Keimer and V. Hinkov
MERGIA Konstantina FP7 9525	Dr Konstantina Mergia Institute of Nuclear Technology and Radiation Protection N.C.S.R. "Demokritos" 15310 Aghia Paraskevi, Athens, Greece	Structural and Magnetic Properties of Ru/Ni Multilayers, Neutron scattering techniques as a tool for non-destructive testing	**Phys. Rev. B (submitted) Vol. 4, No. 1, (2009) 19-33**	K. Mergia, A. Tomou, I. Panagiotopoulos and F. Ott, G. Apostolopoulos, K. Mergia and A.G. Youtsos
UHRIKOVA Daniela FP7 9774	fpharm.uniba.sk	The structural variety of DNA-DPPC-divalent metal cation aggregates: SAXD and SANS study.,	**Eur. Phys. J. Special Topics 167, 191-197 (2009)**	UHRÍKOVÁ D., PULLMANNOVÁ P., KUČERKA N., FUNARI S.S., TEIXEIRA J., BALGAVÝ P
UHRIKOVA Daniela FP7 9774	FP7 9774	Interaction of short-fragmented DNA with phosphatidylcholine bilayers in presence of zinc.,	**Gen. Physiol. Biophys. 28, 146-159 (2009)**	UHRÍKOVÁ D., PULLMANNOVÁ P., BASTOS M., FUNARI S.S., TEIXEIRA J.
UHRIKOVA Daniela FP7 9774	fpharm.uniba.sk	Areas of monounsaturated phosphatidylcholines,	**Biophys. J. 97, 1926-1932 (2009)**	KUČERKA N., GALLOVÁ J., UHRÍKOVÁ D., BALGAVÝ P., BULACU M., MARRINK S.-J., KATSARAS J
JOVARI PAL FP7 9759		Structure of GeSe4-In and GeSe5-In glasses, J. Phys. Condensed Matter, accepted for publication,	**J. Phys. Condensed Matter, accepted for publication**	. Kaban, P. Jóvári, T Petkova, P Petkov, A Stoilova, W Hoyer and B. Beuneu
JOVARI PAL FP7 9759		On the atomic structure of Zr60Cu20Fe20 metallic glass,,	**J. Phys. Condensed Matter, accepted for publication**	I. Kaban, P. Jóvári, M. Stoica, N. Mattern, J. Eckert, W Hoyer, B. Beuneu
JOVARI PAL FP7 9759		Structure of Te-rich Te-Ge-X (X=I, Se, Ga) glasses,	**J. Phys. Condensed Matter, accepted for publication**	P. Jóvári, I. Kaban, Bruno Bureau, Allison Wilhelm, Pierre Lucas, B. Beuneu, D. Zajac,
MALUSZYNSKA Hanna FP7 9840	dr Hanna Maluszynska Faculty of Physics A.Mickiewicz University,	The neutron diffraction study, calorimetry and spontaneous polarization of pyridinium perrhenate at 350 K, 300 K and 100 K,	**accepted for publication in the J. of Physics Condensed Matte**	H. Maluszynska, A. Cousson and P.Czarnecki
R. Mittal et al FP7 9408	Juelich Centre for Neutron Science, IFF, Forschungszentrum Juelich, Outstation at FRM II, Lichtenbergstr. 1, D-85747 Garching, Germany	Measurement of anomalous phonon dispersion of CaFe2As2 single crystals using inelastic neutron scattering	**Pysical Rev. Lett. 102, 217001 (2009)**	R. Mittal, L. Pintschovius, D. Lamago, R. Heid, K-P. Bohnen, D. Reznik, S. L. Chaplot, Y. Su, N. Kumar, S. K. Dhar, A. Thamizhavel, and Th. Brueckel

GeNF highlights

By holography photopolymer grating structures of spatially arranged nanoparticles were produced. SANS measurement first at the GeNF instrument SANS-2 (GKSS) and afterwards at the SANS-1 instrument at SINQ (PSI) showed that these samples have a remarkably efficient diffraction of cold neutrons up to about 50% for effective thicknesses of only 200 µm. The nanoparticle-polymer composites offer the capability to tune or modulate the neutron diffraction efficiency. This is a breakthrough in the search for versatile diffractive elements for cold neutrons and opens up a new perspective for next generation neutron-optical devices like beam splitters or mirrors.

Fally, M.; Klepp, J.; Tomita, Y.; Nakamura, T.; Pruner, C.; Ellabban, M. A.; Rupp, R. A.; Bichler, M.; Drevensek Olenik, I.; Kohlbrecher, J.; Eckerlebe, H.; Lemmel, H.; Rauch, H.; Neutron Optical Beam Splitter from Holographically Structured Nanoparticle-Polymer Composites, Physical Review Letters 105 (2010), 123904.

Water-based ferrofluids (magnetic fluids) are considered to be a potential source of magnetic nanoparticles in brain cancer (glioblastoma) treatment. Small-angle neutron scattering with contrast variation was performed at the SANS-1 instrument at GeNF, using ferrofluids with short-chain-length monocarboxylic acids. The experiments showed - together with the results of transmission electron microscopy studies and magnetization analysis - that the ferrofluids maintain their structure when added to the cancer cell medium. The intracellular accumulations of magnetite from the ferrofluids added to cancer cell cultures as well as its cytotoxicity with respect to human brain cells were investigated. The presented stabilization procedure of water-based ferrofluids is a significant step in the development of magnetic carriers for biomedical applications.

Avdeev, M. V.; Mucha, B.; Lamszus, K.; Vekas, L.; Garamus, V. M.; Feoktystov, A. V.; Marinica, O.; Turcu, R.: Willumeit, R.; Structure and in Vitro Biological Testing of Water-Based Ferrofluids Stabilized by Monocarboxylic Acids, Langmuir 26 (2010), 8503-8509.

BRR highlights

SANS study of the structure of swollen copolymer networks

Ivan Krakovsky, Noémi Székely

The goal of the experiment proposed is SANS study of the structure of block copolymer polymer networks swollen in selective solvents. The solvents used (CD_3OD) and (D_2O) differ in interaction with hydrophobic and hydrophilic blocks built in the networks.

A series of copolymer epoxy networks was prepared by end-linking reaction of *α*,*ω*-diamino terminated poly(oxypropylene)-*b*-poly(oxyethylene)-*b*-poly(oxypropylene) (POP-POE-POP) Jeffamine ED600 (number average of molar mass: $\overline{M}_n$ = ca 600 g/mol), and diglycidyl ether of Bisphenol A propoxylate (PDGEBA) at various initial ratio of reactive groups $r=2[NH_2]_0/[E]_0$.

The networks prepared were swollen to equilibrium in deuterated methanol (CD_3OD) and heavy water (D_2O), respectively. Whereas methanol is good solvent for all the blocks built into the network (POE, POP and PDGEBA), water is good solvent for POE only. Consequently, SANS patterns of the networks swollen in CD_3OD and D_2O differ significantly as illustrated in Fig. 1. In methanol the scattering is governed by frozen and dynamic inhomogeneities, respectively, due to network connectivity and thermal movement of polymer segments. By contrast, in water these contributions to SANS are superimposed by inhomogeneities due to nanophase separation of the system into water-rich

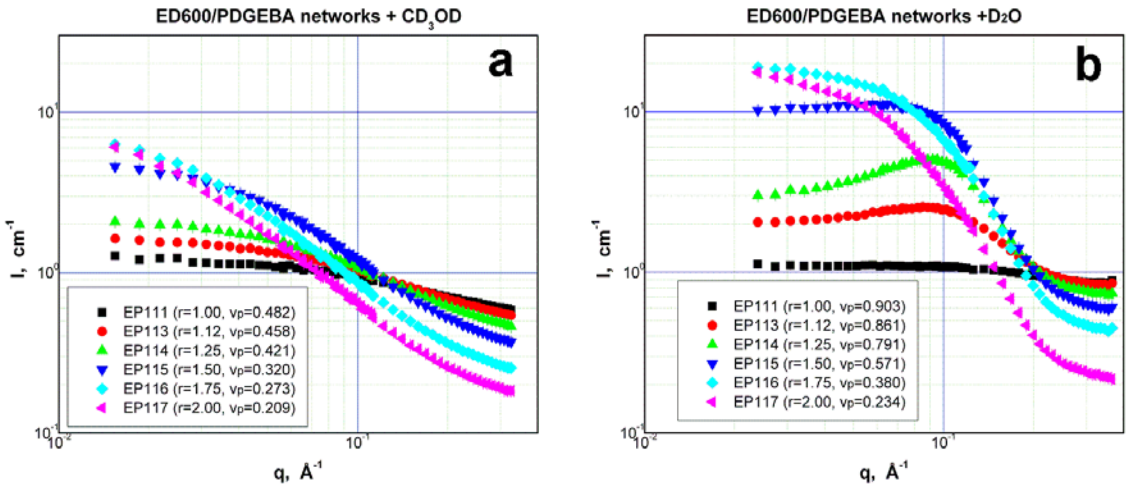

Figure 1 SANS scattering profiles obtained from the epoxy networks swollen to equilibrium in CD_3OD (a) and D_2O (b)at 25 ^oC, v_p denotes polymer volume fraction in swollen networks.

and water-poor domains.

A similar system prepared using much longer POE block in the diamine was investigated by us using SANS previously. SANS patterns obtained from the copolymer epoxy networks swollen in D_2O were fitted well by Percus–Yevick model approximating structure of the system by dispersion of water-poor nanodomains of spherical shape in water-rich matrix. For the system studied in this project, it was found that the Percus-Yevick model fails in fitting SANS data. Another model, namely Teubner–Strey model based on different geometry of nanophase separated structure – locally lamellar order of nanophases – proved to be successful. Characteristic length of the structure as estimated from the position of scattering maxima in Fig. 1 is of the order of tens Å and increases with deviation of the network structure from perfect one expected for r=1.

Formation of the locally lamellar order can be attributed to the conservation of polymer network topology (linear chains of PDGEBA) and shorter length (lower content) of hydrophilic POE blocks in the epoxy networks.

High-temperature neutron diffraction study of the phase transition in a system of lead and bismuth based perovskites

Krezhov Kiril, Erzsébet Sváb

The proposed neutron powder diffraction (NPD) study is focused on determining the details of the crystalline and magnetic structure of $Pb_{0.5}La_{0.5}Fe_{1-x}Mn_xO_3$ ($0 \le x \le 1.0$) and $Pb_{0.5-x}Bi_xLa_{0.5}FeO_3$ ($0<x\le 0.25$), less explored transition metal oxide systems due to difficulties in high-grade sample preparation. $Pb_yLa_{1-y}MnO_3$ ($y \le 0.5$) are ferromagnets with Curie temperature T_C increasing linearly with x to 355 K for x=0.5 and display colossal magnetoresistance (CMR) effects with an MR value of 50% in a field of 5.5 T at 330 K in thin films. Doping of the Mn sites with Fe dramatically alters the material properties leading to wide scope of applications of $Pb_{1-y}La_yFe_{1-x}Mn_xO_3$ such as catalysts, electrode materials in solid oxide fuel cells, exhaust gas sensors, membranes for separation processes etc.

The powder samples with composition very close to the nominal formula (ICP analyses) were successfully produced by a specific solution combustion technique and characterized by thermo-gravimetric/differential thermal analysis (TG/DTA), X-ray diffraction (XRD), magnetic measurements and Mössbauer spectroscopy (MS).

The neutron diffractometers PSD (λ=1.061Å) and MTEST (λ=1.439 Å) were used. The allotted beam time was sufficient to take NPD patterns at 295 K and elevated temperatures on the system $La_{0.5}Pb_{0.5}Fe_xMn_{1-x}O_3$ ($0 \le x \le 1.0$) only. The XRD analyses showed that the samples are single phases with apparently pseudo cubic perovskite structure (Fig.1). The XRD patterns could be indexed in rhombohedral space group R-3c but structure refinements using FullProf produced high χ^2. Susceptibility (Fig.2), TG/DTA and NPD data (Fig.3) evidenced that Néel temperature ($T_N \approx 555$ K, x=0) goes down with increasing x. Simultaneous XRD and NPD Rietveld analyses showed that $La_{0.5}Pb_{0.5}FeO_3$ (x=0) is best described in orthorhombic Pnma space group (Fig.4) in similarity with $LaFeO_3$. The rest crystal structures have Imma symmetry (except R-3c for x=1) as exemplified with Fig.5 for x=0.75. Though Mn^{3+} and Fe^{3+} are with practically identical ionic radius (0.645 Å), the doping affects the crystal structure: there are sizeable lattice deformations reflected in changes in unit cell volume, bond angles and cation-oxygen distances. Furthermore, the magnetic interactions are strongly influenced: the Mn rich compounds (x > 0.5) display ferromagnetism whereas those with high Fe content are canted antiferromagnets. The magnetic structure of x=0 is of G_xF_z-type with main component of the effective magnetic moment on the iron site $S_x = 3.6 \pm 0.2\ \mu_B$. Figs.2 and 6 indicate the phase transition complexity for x=0.5

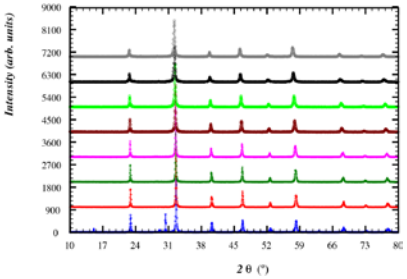

Fig.1

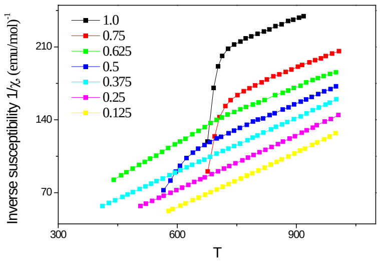

Fig.2

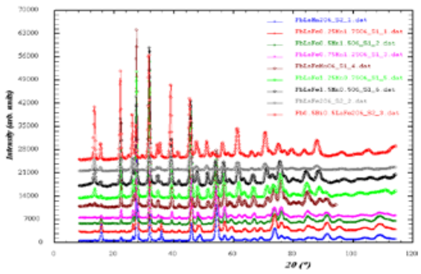

Fig.3

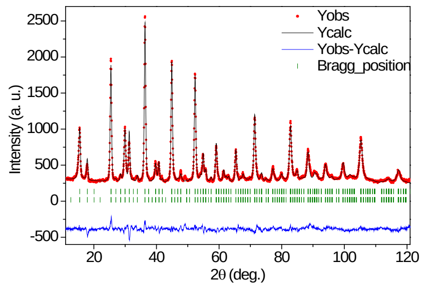

Fig.4

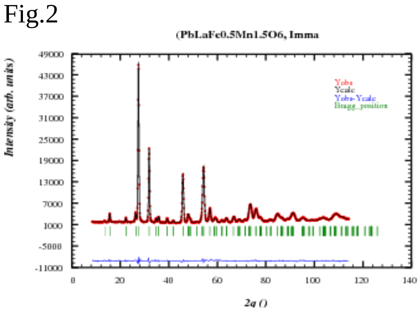

Fig.5

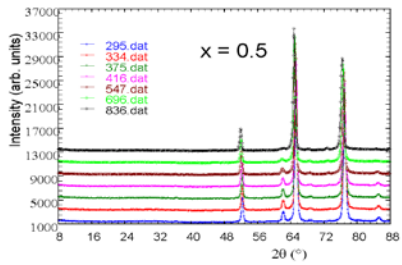

Fig.6

In situ PGAA: a new method to unravel mechanistic details of heterogeneous catalytic processes

Detre Teschner, Zsolt Révay

Prompt Gamma Activation Analysis (PGAA) has been utilized for the analysis of a great variety of materials in many scientific fields, from archaeology through geology to material science determining trace element concentrations especially when no sample preparation is possible. Very recently, PGAA has been further developed by us to analyze reacting components inside a chemical reactor to unravel mechanistic details of heterogeneous catalytic processes. Up to now, two groups of catalytic reactions have been studied, hydrogenation reactions and the so called Deacon reaction for chlorine production. In both cases, the uptake of a reactant fragment (H and Cl, respectively) were investigated under reaction conditions (*in situ*) to correlate the abundance of these species with the activity (and selectivity) of the studied process.

The standard PGAA experiment has been modified in such a way that we placed a continuous-flow catalytic micro-reactor instead of a normal specimen into the neutron beam and recorded the emitted gamma radiation by a Compton suppressed Ge detector. By performing careful reference experiments, we were able to accurately quantify the hydrogen uptake of catalysts (palladium, palladium-based intermetallic compounds as well as complex metallic alloys) in alkyne hydrogenation, being an important group of industrial processes. From the experiments we concluded that – when pure palladium catalysts are used – unselective alkyne hydrogenation proceeds over palladium in the form of hydrogen-saturated β-hydride, whereas selective hydrogenation was independent of the amount of dissolved H in palladium. Since the subsurface hydrogen content is critical for the selectivity, the observed lack of correlation with bulk H can be explained with the occupation of subsurface sites by carbon atoms (in line with our earlier in situ XPS results) disturbing the equilibrium between surface and bulk-dissolved H. When palladium intermetallic compounds (e.g. PdGa, Pd_3Ga_7) were used as catalyst, the modified electronic structure of these materials with filled d-band resulted in the weakening of hydrogen *ad*sorption and no hydrogen was *ab*sorbed in the subsurface and bulk of these materials, giving rise to selective hydrogenation. A similar situation was observed with a noble metal free iron-based complex mixed alloy sample, making it to a cheaper alternative to the Pd system.

The Deacon reaction, oxidation of HCl to produce Cl_2, over RuO_2-based catalysts could be an energy efficient alternative of the NaCl (HCl) electrolysis. We studied the degree of (surface) chlorination by *in situ* PGAA, and observed that adsorbed chlorine poisons the catalyst, decreasing strongly the amount of available surface sites for the reaction. Therefore we can conclude that a modification of the RuO_2 surface to bond Cl weaker can significantly enhance the activity of potential new catalysts.

RID -highlights

All experiments in the FP7 program took place within the past 18 months. No publications have emerged yet resulting from experiments at RID - the delay time between experiment and publication typically is more than two years.

NPI – highlights

Six experiments were supported at NPL from NMI3 sources during PR1. Majority of them were from the fields Engineering & Technology and Materials science, dealing with residual macrostresses and – thanks to the high resolution of NPL diffractometers – also with microstresses.

Besides these experiments, studies in the domain of Life Sciences & Biotech were performed within NMI3. An Israel-German group

(Ben Gurion University of the Negev, Beer-Sheva, Israel, and HZB Berlin, Germany) performed determination of enzyme distributions in novel track-based biosensors (project acronym NPL_2002). Recently, novel biosensor types (e.g. for glucose detection) have been developed where thin enzyme layers (e.g. of glucose oxidase, GOx) are deposited onto the inner walls of etched swift heavy ion tracks in polymers (e.g. PET). In case of contact with an analyte (e.g. glucose), the reaction products enrich in the confined nanopore space, thereby modifying the track´s resistivity via the pH change.

Within NPL_2002 project, the researchers used boron as a marker to control the homogeneity of the enzyme deposition. For this sake, boron depth profiles in the samples at various production stages were determined by Neutron Depth Profiling (NDP). B depth distributions were found that have their highest concentrations slightly below the surface and then gradually decreasing towards greater depths. This reconfirms that the enzymes were really deposited homogeneously within the etched tracks, according to the depth distribution of the etched track wall areas. The observed B surface depletion at 0-0.2 µm stems from the intermediate cleaning procedures during sensor production; excess B precipitates below the surface (0.2-0.8 µm) as expected. The NDP measurements were accompanied by other nuclear analytical techniques such as ITS, PIXE, RBS and current/voltage measurements. The results are mutually consistent. These experiments will be continued with the aim to produce future pulsating track biosensors.

NPL_1010s 2009	B. Ballokova, J. Šaroun, M. Besterci, P. Hvizdoš	Microstructure evaluation of MoSi2 based composite materials by SANS investigations	Metallic Materials	47	refereed paper	375-380
NPL_2002 (2010)	V. Hnatowicz, J. Vacík and D. Fink	Deconvolution of charged particle spectra from neutron depth profiling using Simplex method	REVIEW OF SCIENTIFIC INSTRUMENTS	81	refereed paper	73906

User meetings

ISIS: Main Neutron and Muon User meeting every 1.5 years (last one: April 2009).

User groups hold individual user meetings, e.g.

- Molecular Spectroscopy User Group Meeting (5 March 2010);
- Crystallography User Group Meeting (5-6 November 2009);
- Disordered Materials Data Analysis Workshop (29 Mar – 1 Apr 2010);
- High Field and User meeting (6-7th September 2010)

The ISIS User Committee meets twice per year after the Facility Access Panel Meetings and consists of representatives of the different ISIS user communities.

FRM II/ JCNS: 2nd User Meeting May 25th, 2009, Garching, 100 users, 130 attendees overall, every 1.5 years, next scheduled for October 15th, 2010; not supported by NMI3

PSI: every 2 years PSI organises JUM@P users meeting (not supported by NMI3)

BENSC: Every year HZB organises a joint user meeting for both its large scale facilities BER II and BESSY II. The next meeting is scheduled for 9-10 December 2010.

LLB: Up to date, the LLB has not organised a Users Meeting

GeNF: Since GeNF has a relatively small number of users we do not organize user meetings.

BRR: planned for end of 2010

RID: none

NPL: NPL has no user meetings (substantially lower number of users than at large laboratories