WP1 – Management

Within the last 48 months the project manager took care of the follow-up of delivery status of the different WP obligations. The project manager keeps track of all issues which may arise and need to be discussed in the Board meetings. She also stays in continuous contact with the project officer.

The project manager composed all necessary documents necessary for the periodic & final reports and the two amendments. This included the financial reports and money transfers to beneficiaries.

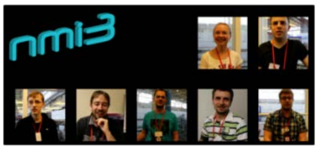
She planned and organized the annual General Assemblies with adjacent Board meetings as well as the Advisory Committee sessions and the review of the School reports (NaMES in WP4). The set-up of the respective agendas and discussion points is in the remits of the project manager, who also proposes and invites the external speakers to the resp. event:

In addition to the very efficient and lean project management, the project manager took care of the industry related activities added in WP1 in the negotiation phase. Three major workshops have been held. The first on ‘Industry as a supplier’ held at the ICNS in Edinburgh, 2013. The second strand was ‘industry as a user’ for which an ‘Industry Advisory Board’ has been set-up. This Board includes industrial representatives using both neutrons and synchrotron facilities. The following two workshops have been done jointly with the homologue lightsoures project CALIPSO. More information is available on *http://nmi3.eu/about-nmi3/industry-.html* .

NETWORKING ACTVITIES

WP2 – Dissemination and Outreach

Communication is essential for raising awareness of research conducted in Europe’s neutron scattering and muon spectroscopy facilities. One of the goals of NMI3-II was to produce articles and videos that could make its scientific activities and achievements more tangible to non-expert publics.



Video teaser of an NMI3 school video.

The website nmi3.eu was an important communication channel among project participants and provides a window to the outside world. Over the years it became a reference to many seeking information about specific neutron techniques.

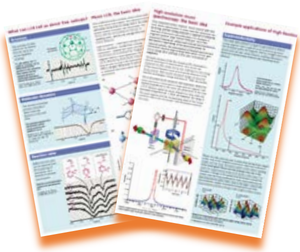
The website Neutronsources.org, which is an initiative of NMI3, was launched to provide information and news on research using neutron beams to a worldwide audience. It is supported by a network of European press officers and thus contains material sent by all neutron sources around the world. There is a page dedicated to each neutron centre and association, news about scientific achievements and events. Those who are new to the field can browse the “Science with Neutrons” page to get to know more about neutrons, their characteristics and applications. Under “Resources” one can learn about projects as well as useful software and tables. On the calendar, you can browse future and past neutron events such as conferences, workshops and schools.

Have you got an idea for a neutron experiment? The website tells you the facilities' deadlines for submission of proposals as well as the operating periods. Are you looking for a job? You might find it on the job tab. The website will remain active after the end of the project.

Group picture at PARI workshop.

Collaboration among press officers of large scale facilities is important to go farther in the promotion and dissemination of the science produced in each of the large scale facilities. Efforts were made within NMI3-II to foster these collaborations by organising regular meetings. The workshop "Public Awareness of Research Infrastructures" in June 2015, which was co-organised by the NMI3 Information Manager, was an interesting opportunity to present expectations, experiences and give examples of work on public relations in each facility.

Would you like to know how neutron scattering contributes to advancing science and technology? The European Neutron Scattering Association published a new brochure on Neutrons for science and technology. It highlights typical work of the academic and industrial user communities to illustrate the scope and potential of neutrons. NMI3-II coordinated the publication. The aim is to distribute copies mainly to scientists and students from other fields, in order to attract new users to the technique.



The development of the muon community focussed on themed workshops on functional materials and soft matter, while publicity leaflets and the muonsources.org website have been created with a view to introducing new user groups to muon technique.

WP3 - E-learning, description of the main S & T results

Introduction

Since experimental neutron scattering is mostly restricted to large-scale facilities, not all students have access to learning the technique at their home institution. Providing a freely accessible e-learning portal for neutron scattering is therefore an important outreach task in order to secure and educate the future users and scientists at neutron scattering facilities. This task and challenge has been taken up by the WP3 partners. The collaboration included people from a broad range of disciplines, from didactics and teaching in physics, through neutron scattering in theory, simulation and experiment to programming and web-design. The aim is to offer online teaching material to university students and their teachers as well as scientists from other fields wanting to learn about neutron scattering techniques.

The Platform

To address this teaching challenge, the WP3 partners have developed and utilized an e-learning portal for neutron scattering under the working title "Virtual Neutrons for Teaching" (VNT) – now fully developed with frontpage available at http://www.e-neutrons.org. - See Figure 1 (left).

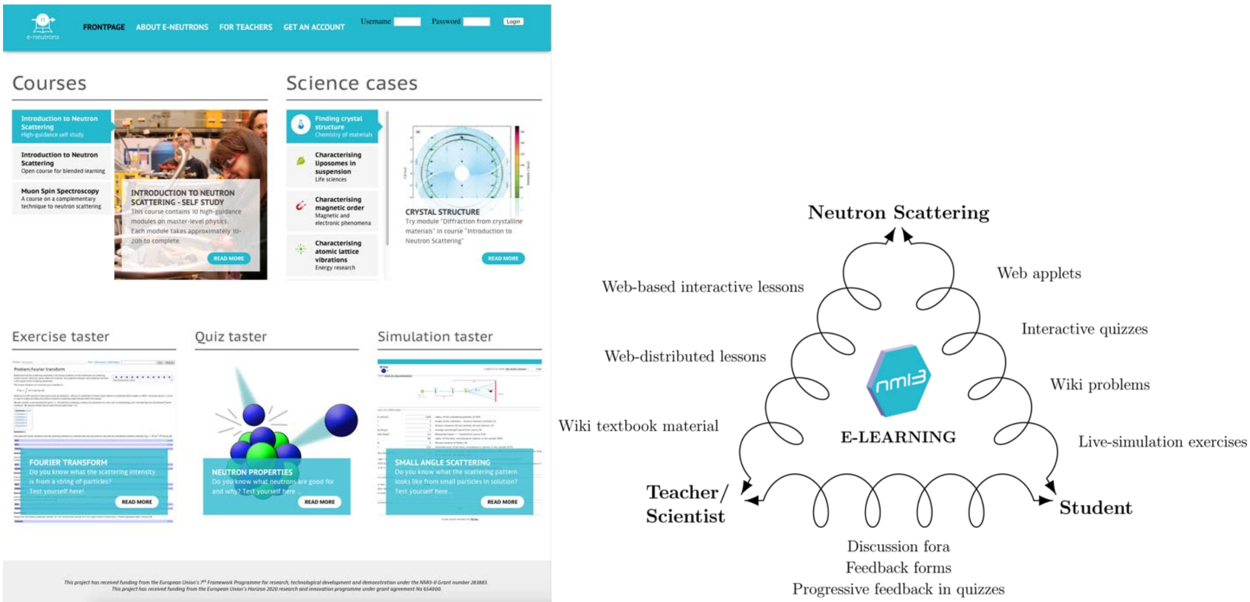


Figure 1:Left: Frontpage from e-neutrons.org. Right: The tools of interaction between the teacher, student and material in the WP3 e-learning project.

Any learning situation can be schematically described in general terms by the interactions between three parts (topic, teacher and student) in the so-called didactic triangle. In a pure e-learning situation the means of interaction are not the same as in a face-to-face class-room situation; some tools are missing while others are gained. The challenge in any learning situation is to balance the interactions on the sides of the triangle in order to optimise the outcome for every student. During the course of the project, key technical and didactical choices have influenced the platform developments. In Figure 1 (right), we have shown schematically some of the neutron e-learning tools we have developed for the platform and how they fit into the didactic triangle.

Once a user is registered at e-neutrons.org, access is granted to the full e-learning platform, made up from three main parts:

1. A "WIKIbook" provided by Mediawiki with various extensions, e.g. for producing mathematical expressions, playing the role of textbook-material – See Figure 2 (left)
2. A Learning Management System (LMS) provided by the Moodle system, providing exercises, quizzes and evaluation – See Figure 2 (right)
3. A web simulator for the McStas neutron instrument simulation program, allowing to perform *virtual neutron scattering experiments* – See Figure 3

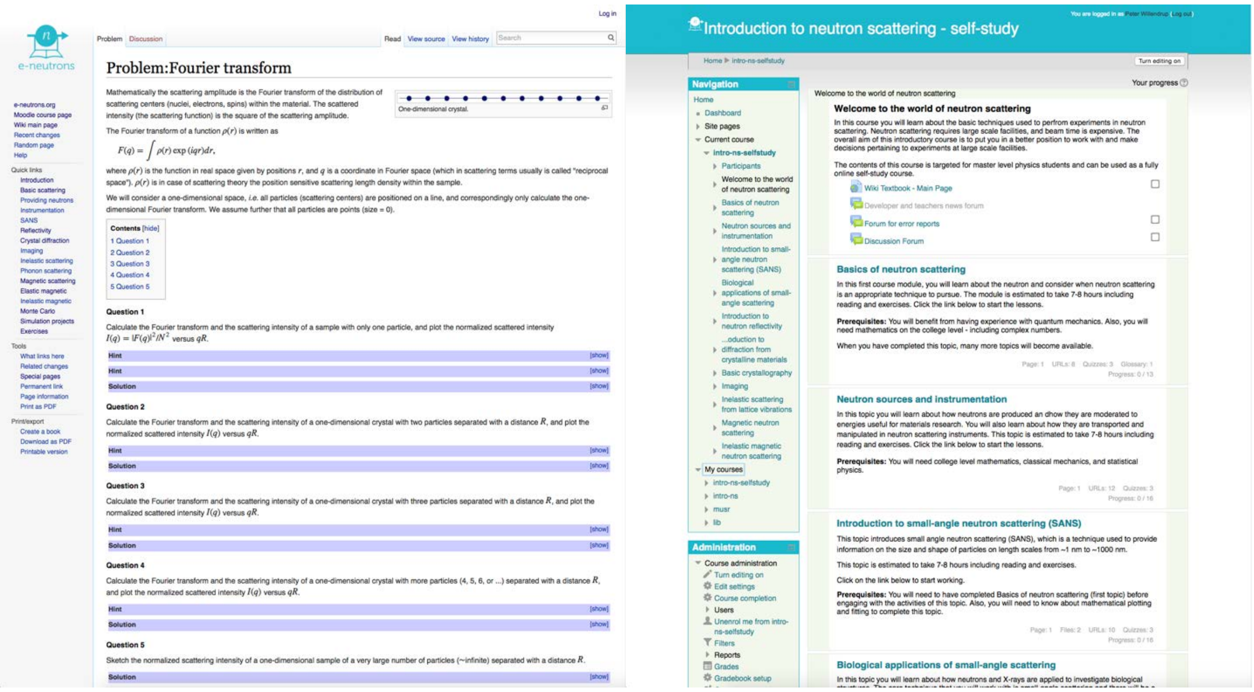


Figure 2 – Left: Textbook example from the WIKIbook - Right: Course material example from the LMS

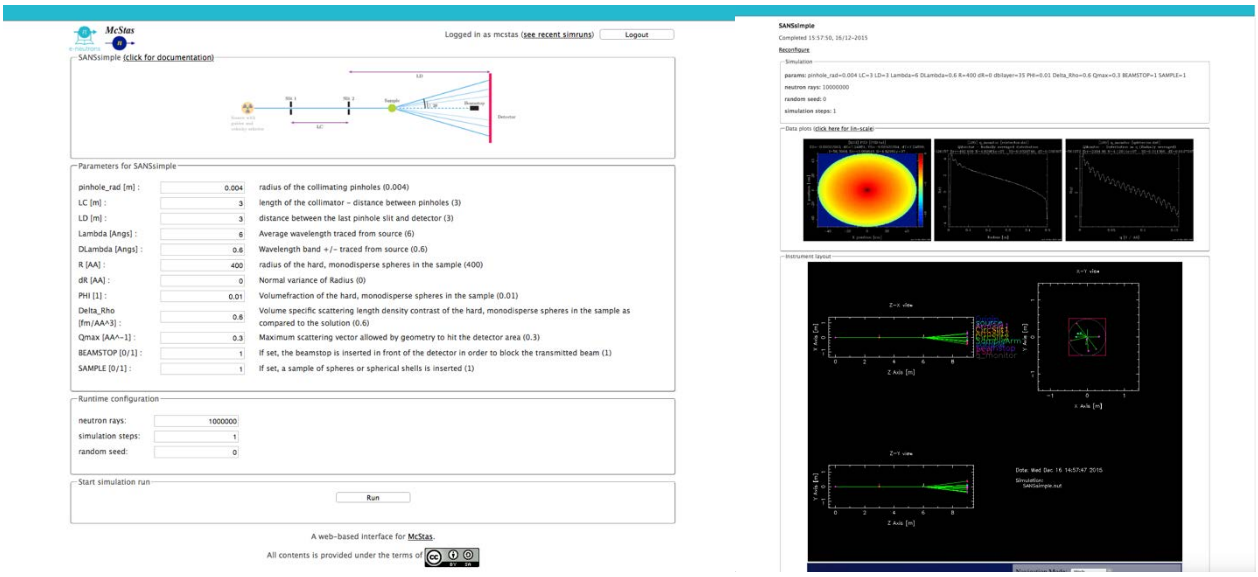


Figure 3 – Left: Configuration page for a virtual SANS instrument - Right: Simulation output from the same virtual instrument

Learning material

We have designed and implemented 10 neutron scattering modules whereof 8 are general introduction to neutron scattering and techniques and 2 are specialised applications in imaging and magnetic neutron scattering. Two courses are constructed from these modules, basically with the same content, but they differ in learning path restrictions and guidance as one course is intended for student self-study. Whereas, the material in the other can be taken in any order and modules skipped, to fit a course in a blended learning setting.

Using the online simulator that contains virtual instruments with samples, the student can tune pre-defined parameters to obtain synthetic data from Monte-Carlo simulations. The resulting data can be analysed like real, measured data. In quiz-lessons connected with some of the instruments the students can explore through theory and virtual experiments, how a neutron scattering technique is used to solve a scientific problem. These quiz-lessons are constructed with the advanced Moodle quiz module which has been used to implement many types of quizzes ranging from student self-tests which can take some minutes up to an hour or two for students to complete, to stand-alone learning modules which take several hours to complete.

Background reading material is made available through the WIKIbook and contains written material and exercises adapted and reworked from coherent and progressive lecture notes collected in an (otherwise unpublished) book by several authors, but with main author and moderator Kim Lefmann.

The tools in the e-learning platform have been thoroughly tested as they were developed in blended learning settings i.e. class-room courses with supplementary material in the e-learning platform. A total number of about 150 students have participated in the tests, mainly in face-to-face courses held in Denmark, Germany and Sweden. User comments in e.g. quiz-replies and focus group interviews have been used to iterate the contents of each module of the courses as well optimise the learning material and activities.

Interoperability of the different software used in the e-learning platform has been ensured through an LDAP based tool developed within this project which from the entry page http://www.e-neutrons.org handles the user account creation and login to each of the three software programmes with the same credentials.

The neutron community are invited to contribute material from schools, pedagogical review papers on methods and techniques, books on neutron scattering which are no longer in print, handbooks and multimedia material via the Library, which is currently implemented as part of the Moodle LMS and upload rights will be granted on request. We have uploaded some key examples as part of WP3. The provision of established books, however, is limited by copyright restrictions. Open source material from schools organised in NaMES (see WP4) and international schools will we added as they become available.

WP4

The achievement is the creation of a distributed Training facility called NaMES - Neutron and Muon European Schools. Collective announcement of a series of schools (brochure and website) ensures their successful occurrence and the refinement of overall interaction and organisation of the schools in the series. Over the four years 17 schools have received support for travel and subsistence cost of the students by NMI3-II. Roughly 1500 students have been supported via the project and hence been made aware of NMI3-II.

The School directors had to provide a detailed financial report in order to make sure that the support is dedicated only to travel and subsistence for students and in special cases for lecturers (in Eastern European countries). All school have put in place a satisfaction survey. The exploitation and hence improvement measures to be taken are in the remits of the respective school organiser.

The NMI3-II Advisory Committee (AC) conducted the first evaluation of the schools in the beginning of 2013. According to this evaluation the schools were judged to be broadly successful. However, in order to attain high, shared standards, recommendations for improving future evaluations of schools have been made. The School reporting rules were refined (WP1) in order to assure a sound assessment of the financial support compared to the total cost of the schools.

The first NaMES schools directors' Synergy Workshop was in Berlin (June 2013), the second NaMES meeting (September 2014) was held in Zaragoza - both satellites to the NMI3 General Assembly. These meetings brought together all schools' directors, some AC members and the NMI3 management. They provided an invaluable forum of discussion for school organization within the NaMES umbrella.

Synergies with the E-learning work package (WP3) have been identified and materials provided.

WP5

Easy and open access to large scale neutron and muon facilities by national and international external scientific users is a general mission of all such public-funded scientific institutions in Europe. Unfortunately the fragmentary structure of the individual user access at the various facilities has been identified as a possible obstacle for the growing user community in Europe. Also, the facilities with large numbers of proposals (e.g. more than 600 per year at TUM) need to spend increasing amounts of time and administrative resources in organizing this task. New large facilities such as the European Spallation Source "ESS" with potential high throughput beam lines may deal with even more severe administrative efforts.

Facing these challenges, of increasing user demand and fragmented access structures, the following objectives have been successfully achieved. The eleven partner facilities offering open access to users, did work in mutual agreement on the tasks defined according to the five objectives, each task being led by one partner.

- Development of a generalized integrated user registration. Technical and legal requirements for a common NMI3 based single electronic user ID to access individual facility digital user office (DUO) systems will be analyzed and the best possible solution will be evaluated and established as a prototype. (Task 5.2)
- Harmonized proposal forms and templates. Forms and templates of proposal submissions at existing DUO applications will be compared and a harmonized proposal template adopted for the individual requirements will be proposed and prepared for implementation. (Task 5.3)
- Web based proposal peer review process. A framework will be developed to allow peer reviewing of submitted proposals within NMI3 web applications for small facilities, which do not operate an individual DUO. (Task 5.4)

- Platforms for cross-source independent beam time access. Platforms to submit proposals for access by the combination of instruments at the NMI3 facilities and platforms for cross-source proposals for the complementary use of instruments, laboratory services or infrastructures using different probes (e.g. neutron, muons, x-rays, facility based AFM or electron microscopy) will be considered and developed. (Task 5.5)

WP6

A clear overview on the existing software landscape for neutron/muon scattering has been established as most of the available neutron and muon software has been identified and evaluated. These have been gathered in a Live DVD, which facilitates software use and testing. The practices employed to develop and maintain the software have been analysed to define a set of recommendations to be used in further projects. The criteria used for the software review are deployment, installation, usability, functionality, maintenance and extendibility. The criteria used for the software practices are related to version control, points of failure, testing, documentation and code duplication.

Among currently developed software, special focus has been given to the Mantid project, which has been developed recently for spallation source instruments at ISIS and SNS. It is investigated to what extent this framework can be used for instruments based at continuous neutron sources. To evaluate the effort required to deliver such functionality, new data loaders have been successfully written for the time-of-flight spectrometers IN4, IN5, IN6 at ILL, MiBemol at LLB, and Focus at SINQ/PSI. A set of existing data treatment algorithms, already available in Mantid, was used, and results were compared satisfactorily with those e.g. of the LAMP software.

A loader for the D33 SANS instrument at ILL was also written. The McStas software was upgraded to write NeXus files readable by Mantid, to account for any virtual instrument model geometry. However, implementing loaders for scanning instruments tends to be more complex in the current Mantid framework. The team will continue investigating beyond the project. Even though the Mantid software provides extensive functionality, some complex and very specific new features may have to be developed as separate, specialized software components.

All deliverables have been published on the NMI3-II web site http://nmi3.eu/about-nmi3/networking/data-analysis-standards.html, and are available to the public, including the produced source code.

JOINT RESEARCH ACTIVITIES

WP17 - Muons

Software Development for Muon Data Analysis

Early in the project we looked at common data analysis procedures, highlighting a requirement for new data analysis tools for processing Avoided Level Crossing spectra, and for carrying out phase-quadrature and rotating reference frame transforms (Fig. 1). These codes were released under the Mantid framework and are now in regular use by the user community.

A parallel study considered how simulation codes might be exploited during data analysis. The ‘Quantum’ package for the simulation of muon spin evolution using the density matrix method was refactored as Python subroutines for execution within the Mantid framework. A number of case studies were developed to illustrate the scope and flexibility of the code (Fig. 1). The potential for using *ab initio* Density Functional Theory methods as an aid to interpreting Avoided Level Crossing spectra was also investigated. Molecular couplings for an example muoniated system were calculated, and used to explore methods for refining these values obtained from simulation. The work demonstrated that further development was required before the technique can be reliably used as a predictive tool in experiments.

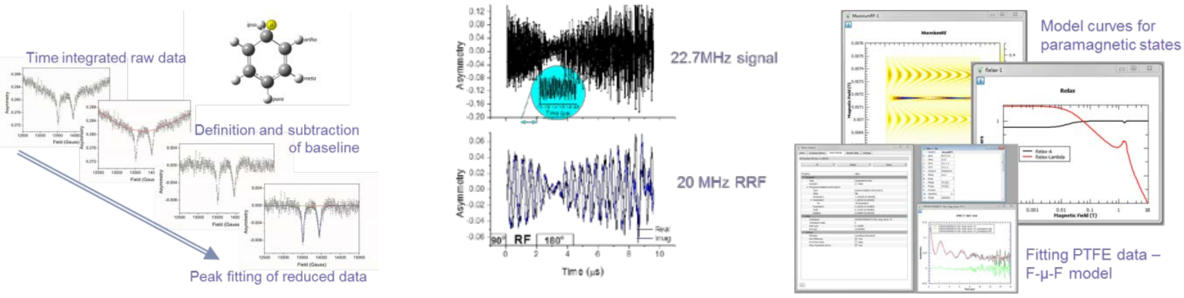


Figure 1: *Workflow for analysis of Avoided Level Crossing data (left), a Rotating Reference Frame transformation of muon spin rotation data (centre) and data modelling carried out using the ‘Quantum’ package.*

Concept Studies for Future Muon Sources

Early discussions with Prof Bob Cywinski, a member of the University of Huddersfield’s International Institute for Accelerator Applications, led to an extended study of target technologies for muon production. The collaboration developed, with Prof Cywinski hosting at a workshop January 2015 (Fig. 2), which brought together facility staff, accelerator scientists and facility users to consider the requirements for next generation muon sources and the scientific problems they might address.

A concept study to investigate the feasibility and research potential of a muon micro-beam (Fig. 2) was also developed as part of the project. The work considered the possibility of carrying out μSR experiments on ~100μm samples, the potential for scanning the sample to investigate inhomogeneities and the possibility of completing parallel measurement of several micro-samples. Very promising results were obtained, with results suggesting a facility could develop a practical micro-beam with relatively modest resources, with greater intensities being possible in the future using more sophisticated focussing and slit systems (akin to electron microscopy).

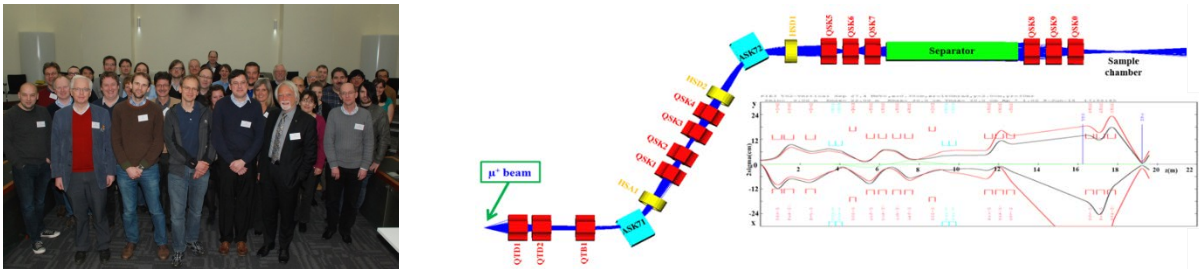


Figure 2: *Attendees at the Future Muon Sources workshop (left) held and the University of Huddersfield, and beam transport modelling for a study investigating the feasibility of producing a muon micro-beam.*

Detector Technologies for Pulsed Muon Sources

Avalanche Photodiodes (APDs) had previously been shown to provide excellent timing resolution that was invariant with magnetic fields. However, their ability to measure the very high instantaneous rates inherent to use at a pulsed muon source was not established. Work within this project developed a systematic study of the performance and operating parameters of APD-based detectors (Fig. 3), enabling the dead time to be properly characterised and compared to equivalent PMT-based systems.

Tests quickly established that the baseline performance of APDs at very high data rates was not ideal because of their extended recovery/dead time (Fig. 3). However, increasing the pixelation greatly improved performance, and further gains were realised by differentiating device output signals before acquisition. For an optimised system, a performance comparable to a photomultiplier-based detector has been realised; however, further work is needed to demonstrate their suitability for building the high density arrays presently being planned for the MuSR and HiFi instruments at ISIS. A fruitful collaboration is developing between the muon groups at the ISIS and J-PARC pulsed sources, with useful discussions ongoing as to how to make best use of these devices in this environment.

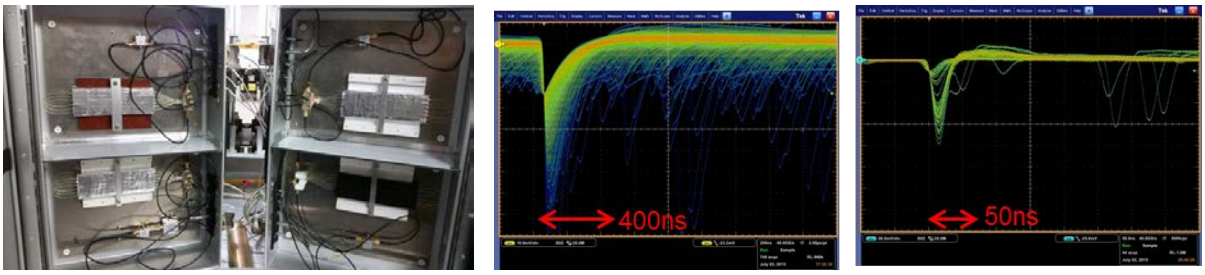


Figure 3: *APD test devices assembled within a light-tight enclosure (left) and signals measured for SensL APDs, comparing the response of the slow (centre) and fast/differentiated outputs. The extended recovery, particularly for the slow output, is immediately apparent.*

WP18 – Neutron imaging

Nano- and micro structures resolved dark-field neutron imaging with grating interferometers (nGI) New set of gratings was manufactured at PSI and TUM (1a). The new gratings allow for increased visibility contrast and therefore for improved performance of the nGI-setup (1b,c). A compact water-cooled 0.4 T electromagnet (1d) was constructed at PSI in cooperation with TUM. To minimize the influence of the magnetic field on the grating setup, the magnet is strongly shielded. A modification of the field distribution inside the magnet is possible by an asymmetric operation of the coils which changes the homogeneous field inside into a distorted configuration. A new nGI setup at ANTARES imaging beamline at FRM-II was constructed with a possibility to rotate all gratings simultaneously around the neutron beam (1b,c). Hence, by an evaluation of the dark-field contrast variation as a function of the rotation angle of the gratings, it is possible to detect anisotropy directions within the microstructure of a sample (1e).

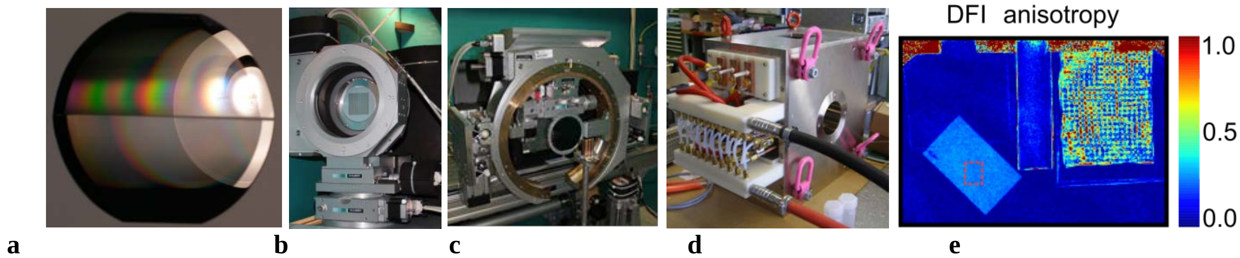
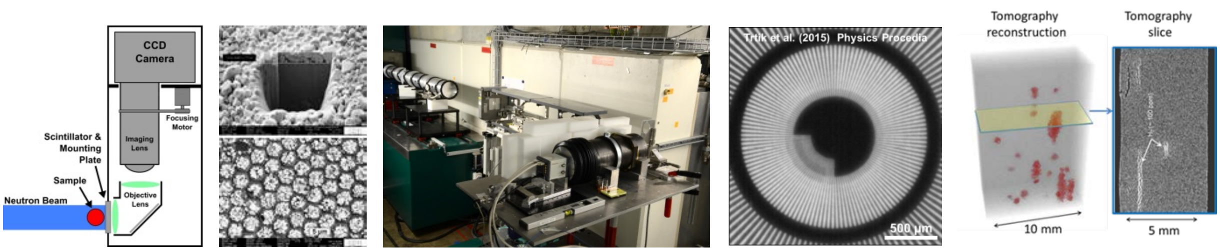


***Figure 1. a)** new gratings manufactured at TUM; **b)c)** photos of the new nGI setup at the ANTARES instrument (FRM-II); **d)** new magnet constructed at PSI; **e)** anisotropy in the microstructural properties of the materials (bottom - Gd µm-grating , middle - copper rod, right - fiberglass material) measured by nGI.*

Direct high resolution neutron imaging

The high-resolution neutron imaging test arrangement is currently being developed at NIAG, PSI in collaboration with HZB under the project entitled "Neutron microscope" (2a). The goal of the project is to develop and implement a dedicated optical system that would allow neutron imaging experiments with spatial resolution below 5 micrometres and within reasonable exposure times. The key element is the development of new high-resolution scintillator screens. Two distinct ways are being followed up– (i) very thin diffuse scintillator based on Gd substances (e.g. $Gd2O2S:Tb3+$) and (ii) micro-structured scintillator screens based on Gd substances (2b). A magnifying optical system was developed. The optical design of the lens has been performed and the first tests were carried out (2c,d). A prototype of new high resolution neutron detector system (2a) at V7/CONRAD-2 instrument at HZB made possible to reach spatial resolution of 15 µm in radiographic images. The optimized detector system opened the possibility of performing tomography experiments (2e) where several hundreds of sample projections are recorded .

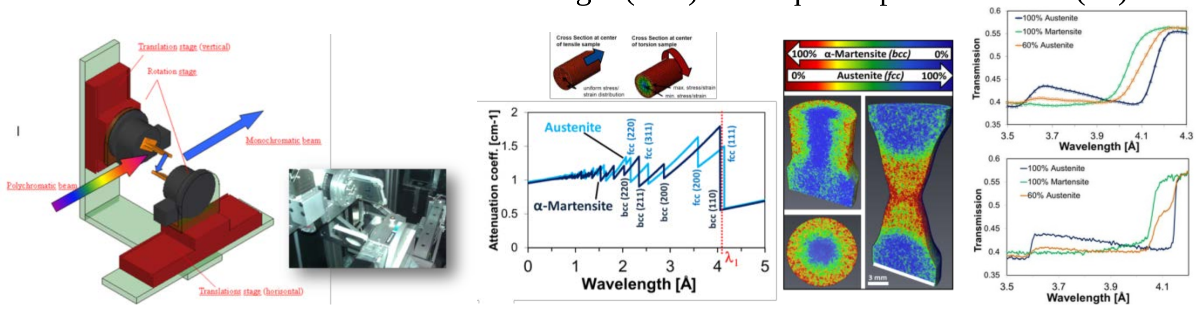


a **b** **c** **d** **e**

Figure 2. a) *high-resolution detector at HZB;* ***b)*** *diffusive (top) and micro-structured (bottom) scintillators;* ***c)*** *high-resolution detector setup at PSI;* ***d)*** *high-resolution neutron image with pixel size 1.5 µm;* ***e)*** *high resolution neutron tomography of hydrogen embrittlement in iron (red=hydrogen).*

Energy-selective neutron imaging

A new energy-selective setup (3a,b) was designed and installed at the neutron imaging instrument CONRAD2 at HZB. The obtained wavelength resolution is in the range of 3 %. The wavelength of the output monochromatic beam can be tuned continuously in the range of 1.5 Å – 6 Å. The setup was used for nondestructive 3D mapping of crystallographic phases within the bulk (centimeter range) of samples with micrometer-scale resolution (3c). The Bragg-edge mapping using continuous neutron sources was extended to Time-of-Flight (ToF) technique on pulsed sources (3d).

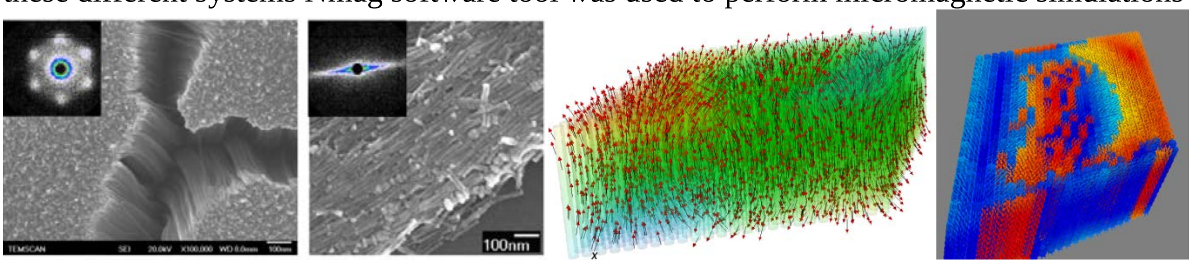


a **b** **c** **d**

Figure 3. a) *double-crystal monochromator installed at the CONRAD-2 instrument at HZB;* ***b)*** *photo of the device;* ***c)*** *Bragg-edge mapping of TRIP steel – 3D crystallographic phase separation;* ***d)*** *Bragg-edge analysis of crystallographic phases in steel by using double crystal monocromator (top) and ToF method (bottom).*

SANS 3D: vectorial magnetic imaging of nano-objects

Polarized SANS measurements have been performed on various systems such as: (i) carpets of Co nanowires deposited on a sapphire substrate (4a), (ii) regular arras of magnetic nanowires deposited in alumina membranes, (iii) aggregates of Co nanowires synthesized by the polyol process (4b). For these different systems Nmag software tool was used to perform micromagnetic simulations (4c,d).

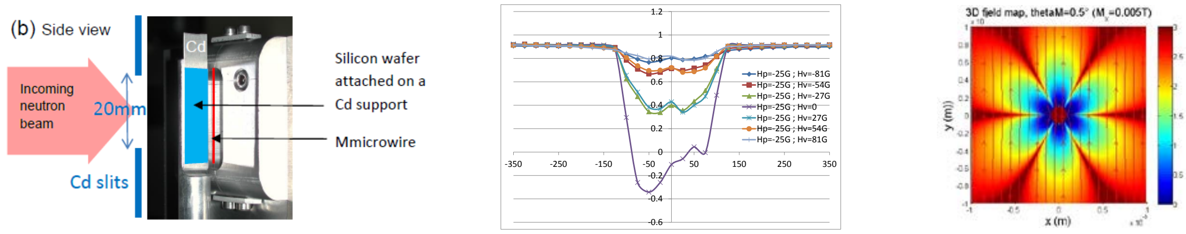


a **b** **c** **d**

Figure 4. a) *Carpet of Co nanowires with the SANS scattering signal;* ***b)*** *aggregates of nanowires with the SANS scattering signal;* ***c,d)*** *Modeling of these systems using micromagnetic simuations of large arrays of nanowires.*

Precession techniques for imaging magnetic structures in thin film systems

Very narrow beams in were produced by using either a silicon reflector (5a) or a neutron wave-guide so that a neutron beam can be scanned across the magnetic wire (5b). Simulations help for data analysis (5c).



a **b** **c**

Figure 5. a) *Micro-beam (20 µm) produced by using a reflection system;* ***b)*** *Neutron precession measurement through a magnetic micro-wire;* ***c)*** *Simulation of a precession measurement through a magnetic microwire.*

WP19 Advanced Methods and Techniques

Sub-mm3 samples for extreme environments

The focusing optics for the upgraded ILL IN5 instrument has been optimized via numerical simulations (McStas) and a particle swarm optimization algorithm appropriate for noisy problems (iFit library). The results confirm that a multi-channel guide is not necessary (Fig. 19.1). For the ThALES 10T magnet entrance channel a focusing guide element has been optimized by a Monte Carlo method (SimRes). The best guide for optimizing the flux at the sample position turned out to be a linear tapered shape.

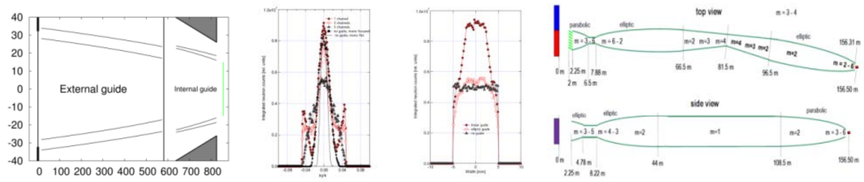


Figure 19.1: Right: vertical profile of the best three-channel guide found for IN5. Middle: performance of a focusing guide element of the ThALES 10T magnet. Right: schematic view of the multipurpose instrument devised for extreme conditions-

The conceptual design of three extreme condition instruments has been achieved. A) A multi-purpose instrument (Helmholtz-Zentrum Berlin) which operates in three modes: diffraction, spectroscopy, and SANS. Such multi-functionality is achieved by a proper design, which consists of a bi-spectral moderator, for cold and thermal neutrons, with a specially designed extraction system; a transport system that incorporates a chopper cascade; etc. Numerical simulations (VITESS) show that its performance and compares favourably with that of existing instruments. B) XtremeD, optimized for high pressure and/or high magnetic field. C) EXPRESSO, a neutron diffractometer optimized for high pressures and the long pulse characteristic of the ESS, will deliver high fluxes at both long and short wavelengths.The design allows direct access to the sample position, and the incorporation of optical probes for in situ pressure measurement (by ruby fluorescence) and ancillary Raman spectroscopy. This set-up also enables a laser heating arrangement of the type used at many synchrotron beam lines.

Spin Echo with Oscillating Intensity for ESS

This joint-research-project is devoted to adaption of the MIEZE technique running on reactor-based instruments like MIRA und RESEDA at the FRM II to the needs of pulsed beams. New resonant spin flipper coils to achieve higher frequencies (resonant spin flip at f = 3.45 MHz) and therefore a higher resolution have been tested (Fig. 19.2). Problems with high currents have been addressed.

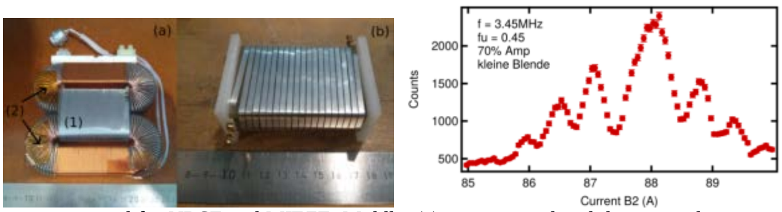


Figure 19.2 Left: the resonance circuit used for NRSE and MIEZE. Middle: (a) conventional coil design used in transversal and longitudinal NRSE; (b) simple coil with low inductivity used for tests. Right: scan of static field B2 at fixed current through resonant flipper coil.

The CASCADE system detector was evaluated, modified and tested for accepting a chopper signal from either a chopper or a synchronization pulse from a pulsed neutron source. Tests were performed at the reactor instruments MIRA and RESEDA of FRM II and at the pulsed beam line CG-1D at HFIR, Oak Ridge National Laboratory (ORNL). The design for the data acquisition and the fitting procedure tested in the pulsed beam line can be clearly chosen as the standard measurement strategy for the planned longitudinal MIEZE spectrometer at ESS. A test of a spin-echo modulated small angle scattering has been successfully performed in the Larmor instrument of ISIS, confirming that there are no significant difficulties in synchronising data collection to the ISIS pulse and no unexpected additional problems.

Choppers for the ESS instrumentation

A chopper concept has been studied with a small high speed motor connected to the rotor by means of an elastic shaft. The system stability at high rotation frequency has been analysed by finite element calculations. The neutronic properties of a single chopper and of a chopper array have been analyzed by means of computations. A (scalable) chopper array with 1% overlapping has been devised which provides the appropriate neutron suppression. Undesirable effects as the suppression of slow neutrons at high rotation frequency have been studied and solutions proposed.

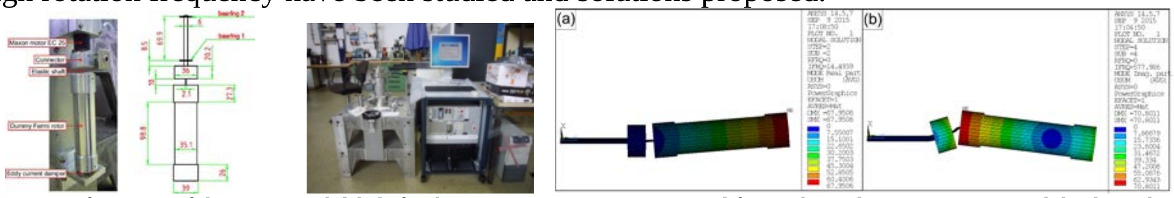


Figure 19.3: Left: picture of the system with labels for the components; Center: test stand for mechanical rotor assessment and the drive electronics rack; Right: results of the stability analysis at high rotation speed.

Polarising all neutrons in a beam

The configuration (Fig. 19.5) is a combination of a neutron polarizing and a neutron transport system, in which both neutron spin states (|↑⟩ or |↓⟩) can be separated, manipulated and re-combined to a beam that can be used for polarized neutron scattering experiments. A super-mirror polarizing cavity comprising two super-mirrors arranged separates the incoming neutron beam into three beams. The lateral beams have polarizations opposite to the central beam. A broadband spin flipper flips the spin state of the neutrons in the central beam. Then the three neutron beams are recombined at the central position of a neutron scattering instrument. Monte Carlo simulations (VITESS) show that the setup has high performance over a broad range of the relevant parameters.

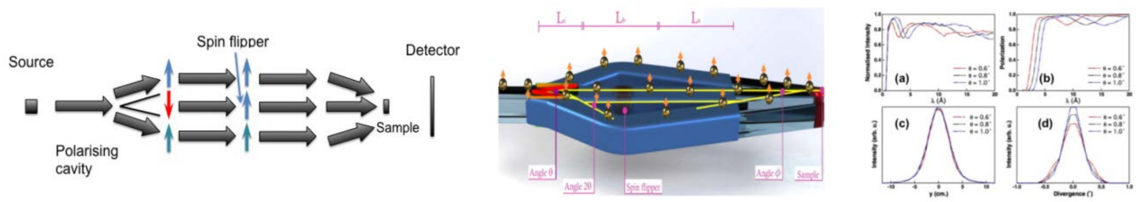


Figure 19.4: Left and center: schematic view of the device. Right: normalised neutron intensity (a), polarisation (b), horizontal beam profile (c) and divergence (d) of the system for three values of the angle θ for the polarising cavity.

WP- 20 Advanced Neutron tools for Soft and Biomaterials

A Platform for model biological membranes

After extraction, purification and analysis of natural lipids from the biomass produced from protein deuteration at the D-Lab facility at ILL, a few neutron reflectivity studies of biomolecules at the surface of natural or deuterated lipids membranes have been then performed. Besides, the method for creating unconstrained, deposited biomembranes on the top of a chemisorbed Self Assembled Monolayer (SAM) of phospholipids on a substrate producing reliable SAM's of effectively 100% coverage is now regularly used as a sample-environment option for user experiments. Significant progresses have been made in the incorporation of Molecular Dynamics calculations for the interpretation of neutron reflectivity curves. Complex membranes from lipids mixed with proteins or peptides, natural ore deuterated, can be better studied by neutron reflectometry thanks to these novel tools, labelled biomaterials and methods.

Kinetic/dynamic measurements in periodic external fields

A new design of observation head for stopped-flow (SF) device has been achieved, allowing a reduction (40%) of the sample volume, and the use of Hellma© cells of different neutron paths. Improvement of the quality of mixing thanks to a new damping grid combined to an automatic push and pumping system (tested) would decrease the duration of mixing and allow measurements of first steps of kinetics after mixing. The SF device, shown in Figure 1, now provides the ability to control the temperature inside the head independently from the temperature of the bath before mixing liquids, and isolates the cell from environmental temperature variations.
A multi-angle dynamic light scattering setup is definitely installed on the Small Angle Neutron Scattering (SANS) spectrometer KWS2 at JCNS. It can be combined with an external commercial static light scattering instrument.

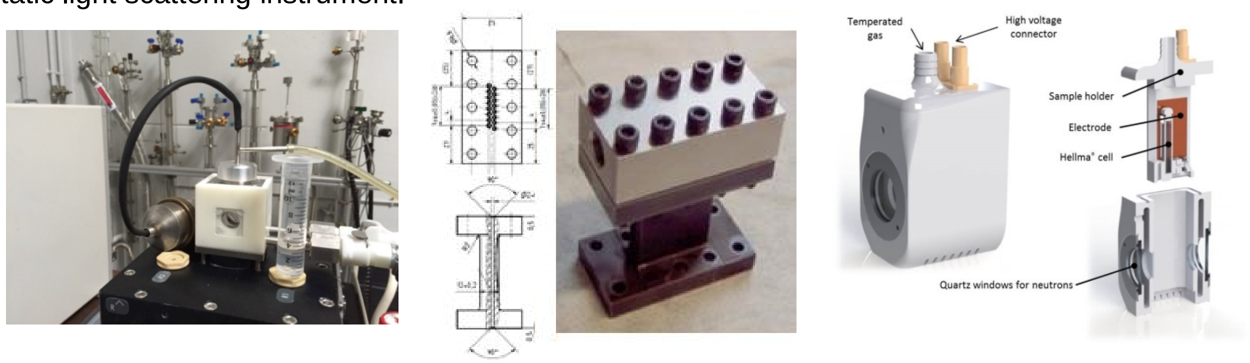


Figure 1. Photograph of the new thermalized observation head mounted on the stopped-flow system at ILL. Design and photograph of a thin walled TiZr pressure cell suitable for high scattering angles optimized for NSE experiments, tested up to 460 MPa for an operation pressure up to 400 MPa. Design of a thermalized electric field cell prototype with electrodes outside the sample in a quartz cell.

Various prototypes of pressure devices for SANS and Neuron Spin Echo (NSE) have been tested and developed during the project. A thin walled TiZr pressure cell dedicated to NSE experiments will allow reaching 400 MPa (see Figure 1) on large sample area (3*3 cm^2). A $TiAl_6V_4$ alloy has been validated as a good material for high performance pressure cell windows (up to 700 MPa in SANS). Design of a separation chamber between the pressure fluid and the sample has been validated up to 700MPa. From experience gained on one prototype with sapphire windows tested up to 450 MPa and validated up to 330 MPa, three versions of pressure cells with sapphire win dows are foreseen: one for NSE experiments up to 50 MPa for 30mm diameter sample's area and two for SANS experiments, up to 500 MPa (with a compromise with respect to the available opening angle or a beam size (intensity) reduction) and up to 300 MPa (without compromise).
Simulations using Finite Element Methods software, COMSOL® Multiphysics, of electric field and air flow have been performed at LLB in order to build a thermalized electric field (EF) cell with electrodes out of the sample cuvette (see Figure 1). The cell body and the sample chamber of a second

prototype of EF cell built during the project are made from PLA by 3D printing. On assembly, the cell was tested successfully with various usual solvents; measurements and simulations of electric field have been compared. Feasibility of thermalization by a simple stream of temperate air flow has been demonstrated.

Humidity chamber

Considerable and collaborative efforts at HZB and ILL have focussed on the design of a humidity cell with a factor of 5 improvements in humidity (i.e. temperature) stabilization. After series of tests on a first prototype chamber in 2014, a second improved version was produced in 2015 (see Figure 2). Highest precision in humidity control is achieved from 0% to 99% relative humidity (r.H.) on both prototypes; special options using Peltier elements (see Figure23) and temperature regulation for fast sample equilibration are required to reach 100% r.H. saturation. The prototype BerILL 1.0 is in HZB user-office since October 2015.

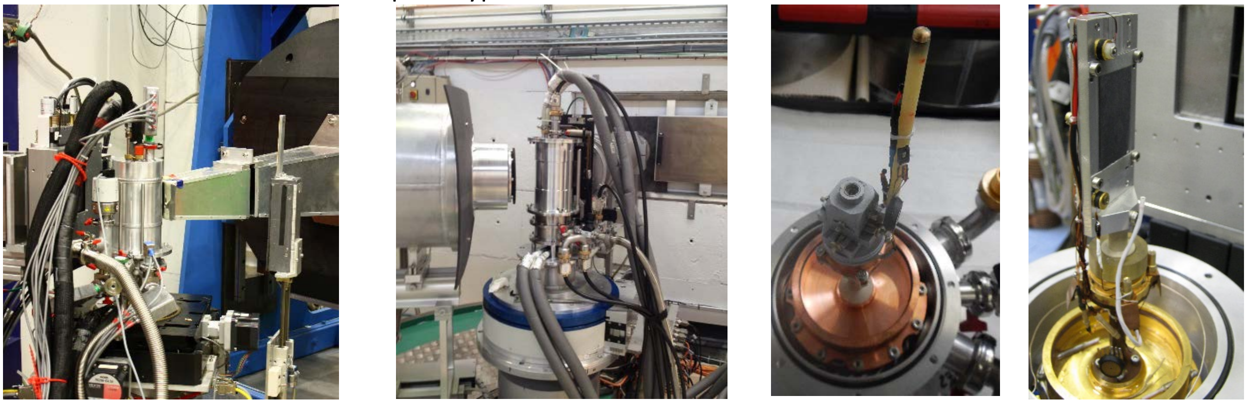


Figure 2. *Humidity chamber BerILL 1.0 at HZB and BerILL 2.0 at ILL Grenoble. Base design of the sample stage with mini goniometer for sample alignment. Peltier to control sample holder T° for highest humidity applications.*

Cryogen free cryostat

A compact and modular cryogen-free cryostat was built with a separate sample space isolation vacuum and a cold head isolation vacuum, allowing the cold volume to be minimized (see Figure 3). Thermal coupling to the cold head is achieved by heat switches to realize fast cool down and warm up. Some elements have been modified after temperature tests. A standardized sample holder providing a pin connection for thermal link and thermometry facilitates sample change and interchange. The sample storage and a robot for sample handling are foreseen to be located at room temperature.

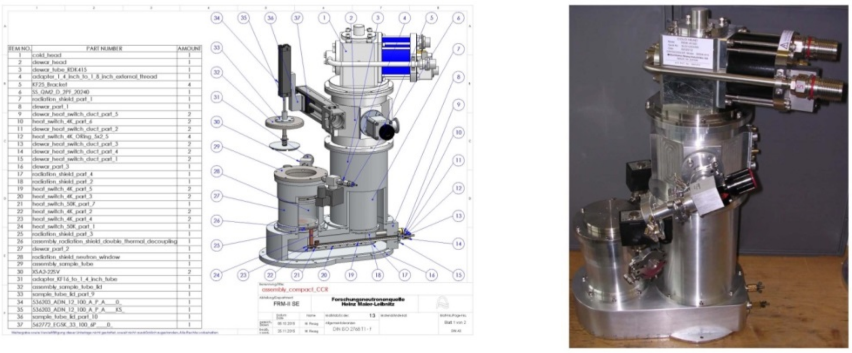


Figure 3. Cryogen-free cryostat: drawings and picture.

WP21 – Detectors

Scintillation detectors

For the scintillation detectors ISIS and Jülich have each developed detectors using ZnS:Ag/^{6}LiF scintillator. The detectors use wavelength shifting (WLS) fibres and multi anode photomultiplier tubes MaPMTs. Different fibre coding, electronics and signal processing have been developed. The final ISIS and Jülich demonstration detectors, shown in Figure 1, have been evaluated. Neutron detection efficiencies and position resolutions can easily be adapted to meet a wide range of applications. The demonstration detectors developed are modular, easy to construct and provide a means of covering large areas in a cost effective manner.

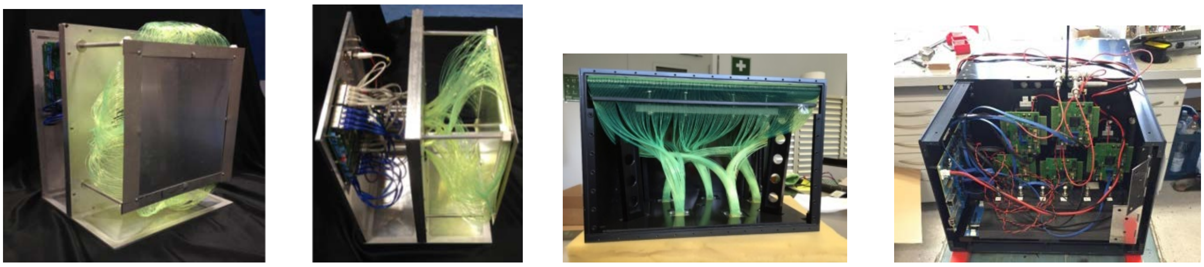


Figure 1. *LHS and LC: ISIS WLS fibre demonstration detector. RC and RHS: Jülich WLS fibre demonstration detector.*

CNR/Perugia has explored the potential of SiPMs for reading out large area neutron scintillation detectors. A system has been developed using up to 7.5 x 7.5 mm^2 GS20 glass scintillators coupled via Plexiglass light guides to a 3 x 3mm^2 SiPMs, see Figure 2. Scalable electronics has been designed and produced and a pulse shape analysis routine has been developed to identify neutron pulses.

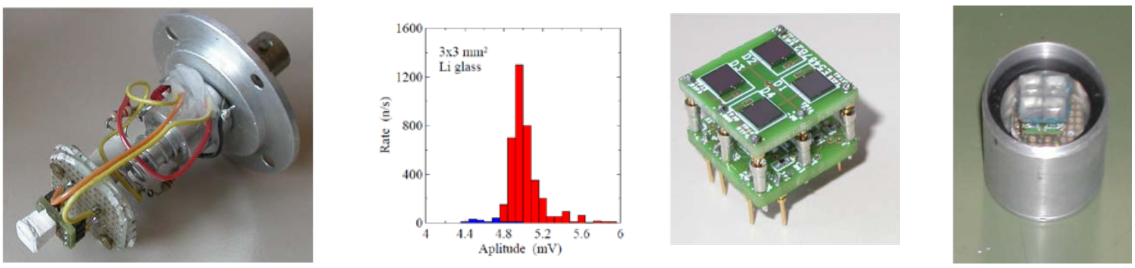


Figure 2. *LHS: Test detector with SiPM connected to GS20 glass scintillator with straight light guides. LC: Pulse height spectrum from a SiPM connected with straight light guide. RC: Four 3 x 3 mm^2 SiPMs mounted on stackable electronics. RHS: Four tapered Plexiglass light guides coupling GS 20 glass scintillator to four SiPMs*

Gas detectors

One of the major challenges in developing gas detectors based on solid ^{10}Boron is the need to deposit ^{10}Boron based layers of ~ 1 μm thickness over large areas. To assess coating quality, TUM and BNC evaluated the performance of $^{10}B_4C$ coatings from a number of different manufacturers produced by both magnetron sputtering and electron beam evaporation, see Figure 3. TUM developed a test detector specifically for this task. Magnetron sputtering is now the accepted standard method of producing $^{10}B_4C$ layers. HZB have studied alternative and potentially faster processes for depositing ^{10}Boron based coatings. They have identified powder spray deposition with a high temperature atmospheric plasma torch as the most promising alternative technique. An experimental system has been developed as shown in Figure 3. A 2D-position sensitive detector has been developed by HZB and BNC to evaluate the quality of these coatings, which is also shown in Figure 3.

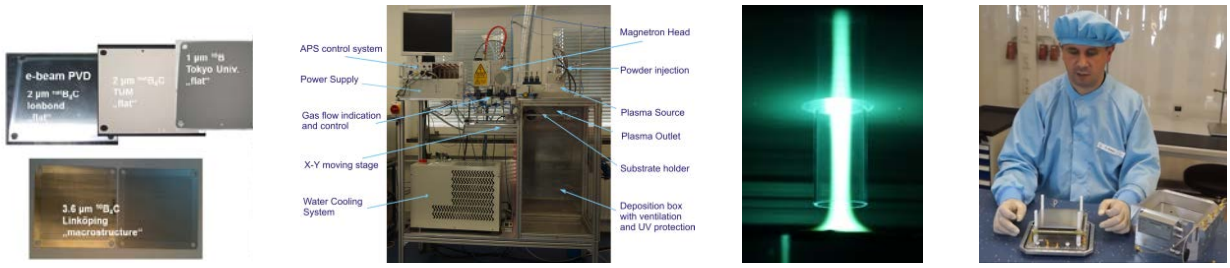


Figure 3. *LHS: Examples of some of the ^{10}Boron coatings evaluated. LC: The Microwave Atmospheric Plasma System at HZB. RC: The plasma jet after ^{10}Boron powder injection. RHS: The 2D detector constructed by BNC and HZB.*

TUM have investigated the "grooved" converters, see Figure 5, in order to reduce the number of $^{10}B_4C$ layers required in a detector, whilst maintaining high neutron detection efficiency. Results show that an increase in detection efficiency of up to ~50% is possible with this design. TUM have developed a concept for a large area gas detector based on these "grooved" converters and multiwire proportional chambers, MWPCs. The concept detector, shown in Figure 4, has an active area of 40 x 40 cm^2 and consists of two MWPCs and four grooved converters. This concept will be developed further by the ESS.

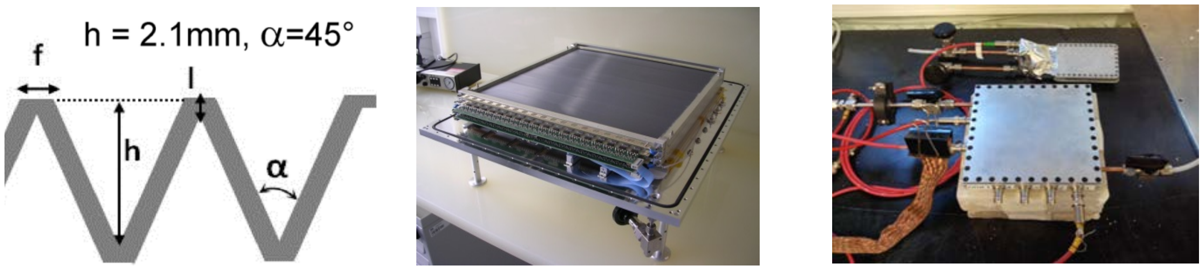


Figure 4. *LHS: Schematic cross section of a "grooved" converter. C: The large area gas detector concept based on "grooved" converters and multiwire proportional counters. RHS: photograph of the concept detector based on a micromegas amplification structure.*

CEA have developed a concept for a large area gas detector based on thin meshes coated with $^{10}B_4C$ on both sides and a bulk micromegas amplification stage. The concept has been extensively simulated to optimise critical construction parameters, operating conditions and neutron detection efficiency. A detector with an active area of 54 x 54 mm^2, shown in Figure 4, has been designed and built to test out this concept.