**Wissenschaftlicher Ergebnisbericht / Scientific Report 2003**

| | |
|---|---|
| Schwerpunkt / main research area | Materie / Matter |
| **FE-Vorhaben / RD project** | **M05 Betrieb und Weiterentwicklung der Neutronenquelle FRJ-2** |
| Institutsbeitrag / institute's contribution | 23105<br>Institut für Festkörperforschung /<br>Institute of Solid State Research (IFF) |
| Verantwortlich / in charge | Prof. Dr. Thomas Brückel T.Brueckel@fz-juelich.de |
| *HGF-Forschungsbereich / Research Field* | *Structure of Matter* |
| *HGF-Programm / Programme* | ***Large Scale Facilities for Research with Photons, Neutrons and Ions*** |
| *HGF-Thema / Topic* | *Neutrons* |
| Internet | www.fz-juelich.de/scientific-report |

**Detailergebnisse / Details**

# Progress report of the new NSE spectrometer for the SNS

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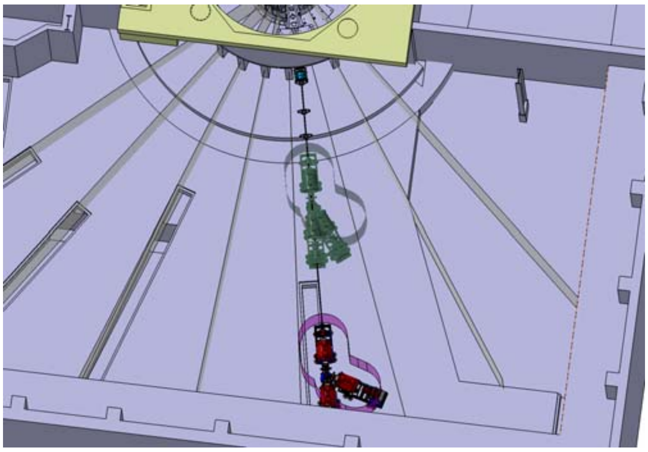
To build a beyond state of the art NSE spectrometer is the major challenge of our recent research and development program. The instrument will be the best of its class instrument both with respect to highest resolution up to a Fouriertime of about τ=1μs and huge dynamic range of more than six decades in time. This will be achieved by two key technologies, superconducting main precession coils and highest current carrying correction elements. While it has been shown that superconducting coils can be used the correction elements are still under development. Furtheron the dynamic range can be expanded by an additional decade in time with the usage of radio frequency π/2 - flippers. In addition and to optimize the useable wavelengths frame and the maximum scattering angle, Q – range respectively the instrument should be variable with a detector to moderator distance from 18m up to 28m. Also the instrument should be equipped with a so called intensity modulated NSE option to study materials which normally depolarize the beam. The instrument concept has been presented in spring 2003 and beamline 15 of the uprising new spallation neutron source in Oak Ridge has been reserved.

One major role of the instrument will be to supply a unique facility to analyze the dynamics contained in the SANS intensity and thereby to unravel molecular motions and mobilities at the nano- and mesoscopic level. A feature which is of utmost relevance for "soft matter" problems that occur in research fields as molecular rheology of polymer melts, related phenomena in networks and rubbers, interface fluctuations in complex fluids, polyelectrolytes, transport in polymeric electrolytes and gel systems. In biophysics the molecular dynamics of proteins, phospholipid membranes and other biomolecules is about to gain in importance. In particular the grown up and still improving facilities of molecular dynamics calculations that meanwhile extend into the multi nanosecond time domain allow for a detailed comparison with neutron scattering results. On the other hand, the longest Fourier times of the proposed instrument will establish a direct link to the light scattering (DLS) domain. However, with all the additional possibilities of the game of contrast variation that is so unique for neutrons.

During the last year the final layout and concept has been worked out and the instrument has been presented at the EFAC meeting in spring 2003 at the SNS. As a result beamline 15 has been assigned to the instrument. The instrument is shown in Fig. 1 at two different positions.

The proposed NSE instrument is of the original generic IN11 kind, which is the technique with the largest potential to extend the resolution beyond current limits. The new instrument will have the following worldwide unique features:

- Ultra high resolution: $\tau_{max}$=1μs (Δħω= 0.7neV).
- Huge dynamical range extending at least up to 1:$10^6$.
- Scattering angle up to 63°.
- Position sensitive area detector with broad detection region.
- Field compensation and magnetic shielding.
- Optional intensity-modulated mode.



Fiq. 1: The upper drawing shows the instrument on beamline 15 of the SNS experimental hall. It wil be possible to operate the instrument at distances from 18m to 28m using a four chopper system.

A moderator detector distance of 18m yields a wavelengths frame width of Δλ=0.366nm. However this distance may be made variable up to 28m with a four chopper system to trade flux versat long wavelengths versus scattering angle. At 18m the maximum scattering angle is limited to 28° and at 28m to 63° while the usable wavelength frame changes from Δλ=3.66Å to Δλ=2.35Å. The resolution of $\tau_{max}$=1μs shall be obtained for λ>1.8nm with a field integral J>1Tm. In addition due to the λ separation by time – of – flight (TOF) the wavelength dependent part of the Q-resolution is an order of magnitude better than at reactor instruments. Exploiting that the Fourier time $\tau \sim \lambda^3$ a subsequent use of various frames covering 0.3<λ/nm<1.83 in combination with variation of the magnetic field (integral) by a factor >1000 a huge dynamical range of more than six decades in time is achieved. This dynamic range can be further extended to approximately 0.2ps with the combination of NRSE with the generic NSE technique operating the $\pi/2$ - flippers with radio frequency [2]. By automatic set-up procedures the change of wavelength frames will be a routine operation with negligible time delay. The inherent change of $Q(\lambda)\sim 1/\lambda$ together with $\tau\sim\lambda^3$ fortunately complies with the usual dispersion of relaxation rates $\Gamma\sim Q^2\ldots Q^4$. An area-sensitive fast detector of 30cm diameter will cover a solid angle of $\Delta\Omega>4°\times 4°$ and assures efficient data collection rate. The magnetic stray field of the main coils is compensated down to $1..1.5\times 10^{-4}$T in 1.5m distance. Thereby it becomes possible to enclose the instrument area by a magnetic shielding which ensures a stable and reliable operation. Here further theoretical calculations are required. The latter also depends on a rigid mechanical design which enhances the stability. The thus achieved signal stability is an utterly important but often overlooked quality. Additional flippers (ferromagnetic mode) and polarizer/analysers (intensity modulated mode) will offer the unique opportunity to perform a polarization analysis of the scattering from magnetic samples, to deal with depolarising samples [3], or separate coherent and spin-incoherent scattering.

The placement of components along the beam line will be described below. The neutron guide section starts with the shutter insert at about 2.5m distance from the cold coupled moderator. Guides shall be Ni-coated and have a cross section of 4cm (width) x 8cm (height). A chopper system consisting of four choppers selects the required wavelength frame. Between the first and second chopper a short polarizing bender is located that introduces a bend of the beam line of 3.5° out of the direct line of sight. For different wavelength ranges –each covering several frames- different solid state microbenders are required [4]. For that purpose 2-3 benders are situated in a revolver - system. A fourth position of the revolver (length ~0.5m) serves as auxiliary shutter. After the benders a guide field in the neutron guide field preserves the polarization. Between the last (3rd) chopper the guide field is rotated from vertical to longitudinal direction. The expected flux on the sample has been determined using the VITESS Monte-Carlo code [5]. It has been shown that at lowest wavelengths a reasonable sample flux of about $10^8$n/cm$^2$s and at highest wavelengths of about $5*10^5$n/cm$^2$s could be achieved in the wavelengths range between $0.3\text{nm}<\lambda<2.2\text{nm}$. Thus a respectable flux for most practical usage will be obtained. The time averaged intensity on the sample will be comparable respectively higher than the flux at the high flux ILL instrument IN11.

The Fourier time of 1μs requires the use of long wavelengths up to 1.8 nm in combination with a large magnetic precession field (J>1Tm). As the intensity modulated NSE absorbs a factor of about 100 neutrons due to the in beam devices the maximum achievable wavelength with reasonable flux is limited to 0.8nm.

The “primary” shielding sector around the neutron guide ends at about 10…11m. The following NSE area is enclosed by a combined magnetic and radiation shielding. The functional components are located on three separate mechanical carriers: first arm, sample stage and second arm. The carriers move on air pads on a special floor (tanzboden). The main solenoids -one on each arm- consist each of two concentric cylindrical superconducting coils that provide high field integrals in combination with compensation for lowest stray field [1]. Flippers limit the precession paths. They are operated with current ramps that are adapted to the time varying wavelength within the selected frame. For low Q-SANS an optional converging collimator in front of the sample is foreseen.

After traversing the last $\pi/2$-flipper the neutrons enter a combination of background suppression collimator and analyser, before those with the right final spin polarization hit the detector. The scattering arm has to be rotated around the sample position in order to realize a reasonable momentum transfer (Q) range. This determines the lateral space requirements. The instrument has to be restricted to a maximum scattering angle of about 63° in order not to violate its sector boundaries. The thus usable Q – space is $0.0025\ \text{Å}^{-1}<Q<2.1\text{Å}^{-1}$.

To summarize: During the last year the instrument layout and concept has been finished and subsequently presented at the EFAC meeting 2003 at the SNS. As a result beamline 15 has been reserved for the instrument. This novel NSE instrument will be unique and best-of-its class both in resolution up to 0.7neV and dynamic range over more than six decades. Compared to single detector NSE instruments it will accept a significantly larger solid angle. Therefore, the effective data rate will gain an additional factor of 5 in addition with the estimated time averaged sample flux of $10^7$ n/cm$^2$s around $\lambda$=1nm. This yields to the highest available data accumulation rate. As additional and important extra quality the wavelength distribution width at any time is well below 0.5%. Thereby the resolution in momentum transfer increases significantly compared to reactor instruments with 10% or more wavelength distribution width. The optional intensity modulated NSE option open the window to magnetic fluctuations. This instrument it will open up new experimental possibilities and qualities in soft matter research as well as in the field of magnetism. The instruments costs have been proposed for funding and decision is expected in 2004.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# A New Method of Vector Polarization Analysis for Neutron Scattering

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Polarized neutron scattering is a unique technique to reveal magnetic structures and excitations. We have developed a new method using precessing neutron polarization, which achieves full vector polarization analysis. This method overcomes problems and limitations of current methods based on zero-field techniques. Furthermore, it allows to analyze the scattering simultaneously for all scattering angles and energy transfers.

The neutron's magnetic moment is an ideal probe to study magnetic structures and excitations in condensed matter physics. In general, scattering cross-sections for magnetic scattering depend on the direction of the polarisation of the incident neutron beam with respect to (i) the scattering vector **Q** and (ii) the direction of the magnetic moments in the sample. Two simple rules can be established: First, only the component of the magnetic moments which is perpendicular to **Q** contributes to scattering of neutrons. Second, the component of the initial neutron polarization, which is perpendicular to the magnetic moments in the sample, changes sign upon scattering. From these considerations it is apparent that in particular polarized neutron scattering and polarization analysis is a technique to identify uniquely magnetic structures and/or excitations. Therefore, however, it is in principle necessary to observe and analyse arbitrary rotations of the neutron polarization in the scattering experiment, which is a difficult and time consuming task. It requires the twofold determination of a three by three matrix $P_{if}$ given by the vectors of the initial and final polarization $\mathbf{P}_i$ and $\mathbf{P}_f$ respectively; twofold for parallel and anti-parallel orientations of the polarisation, *i. e.* the so-called non-spin flip and spin-flip scattering processes. All current methods[1–4] for this purpose of vector polarisation analysis are essentially based on zero field techniques. Their idea is to avoid any uncontrolled precession of the neutron polarisation. However, as already pointed out by Schärpf[5], a vector polarisation analysis is possible with precessing polarisation. Schärpf's idea gave the inspiration for a new method for vector polarisation analysis which differs from his original proposal in using the precessing mode for the *initial* neutron polarisation[6]. This new method allows to measure and analyse simultaneously the polarisation of scattered neutrons for all scattering angles and energy transfers. This principle has of course a decisive advantage for multi-detector instruments and time-of-flight machines. In particular, studies of diffuse, inelastic magnetic scattering may become now an achievable task. Furthermore, the method fits perfectly to the needs of modern instrumentation at pulsed neutron spallation sources.

The method has been successfully employed on the DNS instrument, a neutron time-of-flight spectrometer for diffuse scattering with polarisation analysis. Similarly to the D7 instrument at ILL Grenoble, it has been equipped with neutron polarizers and analyzers covering a wide angular range. A polarizing supermirror bender placed in the incident beam produces polarized neutrons perpendicular to the horizontal scattering plane. The polarisation is kept in a vertical guide field but can be switched upside down by a "$\pi$-flipper"; here neutrons perform half of a Larmor-precession in the field of a rectangular current coil. A set of further coils around the sample position allows to change and to tune the magnetic field arbitrarily from the direction of the guide field. For sufficiently strong fields the neutron beam polarisation can follow the spatially varying magnetic field. In usual experiments for instance on paramagnetic samples this set-up allows to measure spin-flip and non-spin flip scattering for orthogonal directions, say x,y,z, which determines the diagonal of the matrix $P_{if}$, $P_{if}^{xx}$, $P_{if}^{yy}$, and $P_{if}^{zz}$. One may note that the new method does not require new experimental devices. To explain the method in detail, we consider how one can measure an off-diagonal matrix element of $P_{if}$, say $P_{if}^{xy}$ which means a rotation of the polarisation from x-direction for initial neutrons to y-direction for final neutrons. Therefore, the magnetic field should be parallel to y, so that this final polarisation component $P_f^y$ will not precess and can easily be analysed by the final polariser. The initial polarisation has to be set to $P_i^x$ at the sample position. Since it is perpendicular to the magnetic field $B = (0, B^y, 0)$, it will be precessing. Therefore, the "flipper" is set to impose only a $\pi/2$ rotation on the initial neutron polarisation. The absolute precession angle, which the neutron spins perform on their way from the flipper to the sample, is determined by the path integral of the magnetic field. It is tuned by the magnetic field strength of the y-coils around the sample. Using a crystal with well-known magnetic properties the absolute precession angle can now be calibrated as a function of the magnetic field.

This situation has been simulated and is displayed in Fig.1. In our experiment we have chosen the antiferromagnet $MnF_2$ to verify the principle. Magnetic moments in $MnF_2$ point along the $\pm$c-axis. Therefore, if the orientation of the c-axis is chosen to be bisecting between x and y, the neutron polarisation will flip from $P_i^x$ to $P_f^y$

during the scattering process. The first results are shown in Fig.2. The maxima of intensity versus magnetic field strength are found for $\mathbf{P}_i$ parallel to x, minima for $\mathbf{P}_i$ anti-parallel to x, and the points of zero curvature are related to $\mathbf{P}_i$ either parallel or anti-parallel to z. One may note that the flipper has been placed close to the sample, because the wave-length spread of the incoming neutrons causes a dephasing and only a few precessions are tolerable. In practice, it is important to correct the "flipper"-currents to the changes that stem from the surrounding fields. Recently, by optimising fields and corrections, we have achieved much improved results. As shown in Fig. 3, the ratios between minimum and maximum intensities for such off-diagonal elements are now much higher and almost of the same quality as for the diagonal terms of $P_{if}$ that are conventionally determined without precession techniques.

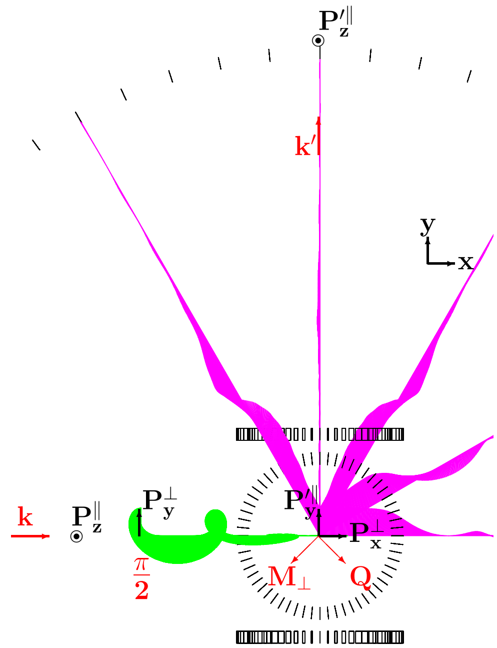


FIG. 1: Simulation of precessing neutron polarization analysis of the off-diagonal element $P_{xy}$ for typical parameters of the DNS instrument.

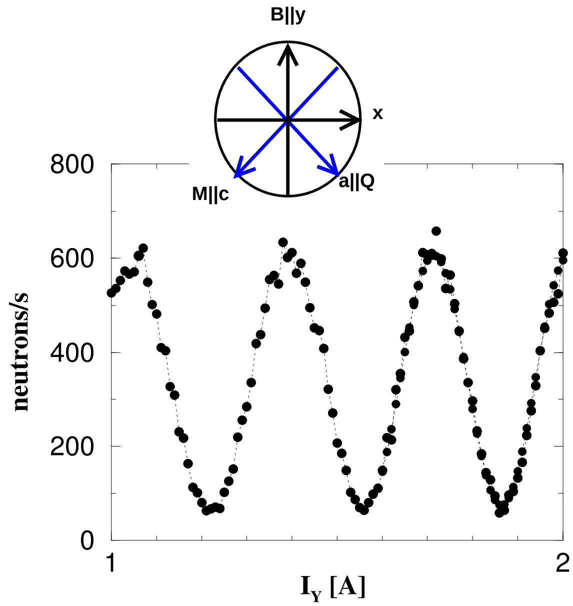


FIG. 2: First results of magnetic scattering of the (001) Bragg reflection of $MnF_2$ measured with a precessing incident polarisation perpendicular to $B^y$. Maxima (minima) occur for a rotation of $P_i^x$ to $P_f^y$ ( $P_f^{-y}$).

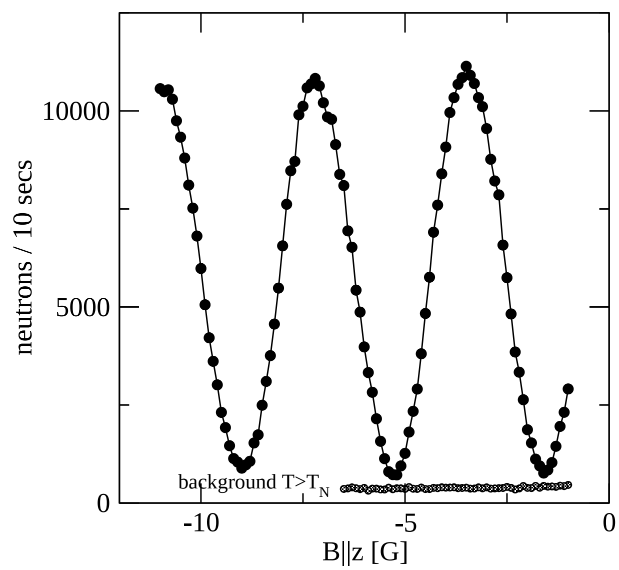


FIG. 3: Magnetic scattering of the (001) Bragg reflection of $MnF_2$ measured with an incindent polarisation precessing perpendicular to $B^z$. Here the c-axis is inclined by 45 °. Maxima (minima) occur for a rotation of $P_i \perp a$ to $P_f^z$

We gratefully acknowledge M. Monkenbusch (IFF) for software to simulate changes of the neutron polarisation in scattering experiments.


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