

SWISS NEUTRON NEWS



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Swiss Neutron Scattering Society

Editorial:

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Cover illustration

The construction of the SINQ guide hall extension at the end of November 2003. In October the construction has started. It is foreseen to complete the new hall up to the end of the 2004 shutdown, such that it is ready for occupancy by then. The guide hall extension will host the new backscattering spectrometer MARS, sample preparation and electronic laboratories as well as space for computing facilities for the users.

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The President's Page



Dear members,

in my past few editorials I have been focusing on the rise and fall of the ESS project and its role in the planning of the future of the access of our community to the international neutron facilities. It is clear that this theme will again be a vital issue in our next general assembly on January 22, where we will have to discuss the possible alternatives to the ESS such as a participation at the American spallation source SNS. This discussion has already been started some months ago with the survey and questionnaire that you have all received.

However, upon all these discussions about the neutron sources of the future and the best way of making them fully accessible to our Swiss user community we should also not forget the tremendous achievements at SINQ that have made this such a success story in the last few years. We have all witnessed the considerable improvements of the source and all the instruments, and I would like to take this opportunity to thank all the instrument responsables for their enormous effort and their commitment that have made it a real pleasure to work at SINQ. It is clear that the successful proposal for the participation of SINQ in the 5th EU framework program (FP5) has been very important for the the success of SINQ as a truly international neutron source, and it is of course important that it has been possible to secure the support within the new FP6 program. The high annual number of proposals and the significant overbooking of the entire instrument suite demonstrate the attractiveness and competitiveness of SINQ, and it is obvious that we all profit from the international character and the high quality research that is performed there.

Those of us that have recently been doing experiments at SINQ have seen another direct sign of the commitment of PSI to constantly improve the conditions for our users. The construction of the extension of the neutron guide hall with its laboratories is well underway, and I do look forward to the moment when we will be able to use the new IT facilities and the chemistry laboratory that will make such a difference in particular for the soft matter and biology community. Moreover, with the new spec-

trometers MARS and TNT the PSI complements the already attractive list of instruments with two new highlights, and the expected performance of both will certainly make those very competitive instruments that further add to the attractiveness of SINQ. While the future of neutron scattering for the coming generation of young and talented scientists may be somewhat endangered by the political decisions and developments on a European level, it is clear that we are enjoying a highly successful situation at our home base and, thanks to the combined effort of the PSI and the continuous support by the Swiss Federal Office for Education and Research ('Bundesamt für Bildung und Wissenschaft, BBW') we can look forward to a bright future for neutron scattering in Switzerland.

Peter Schurtenberger



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All members of the Swiss Neutron Scattering Society are cordially invited to participate in the

2004 General Assembly
Thursday, 22/01/2004, 17:00 – 18:30
Paul Scherrer Institut, main auditorium

Agenda:

1. Welcome
2. Minutes of the General Assembly 2003
3. Annual Report of the Chairman
4. Annual Report of the Treasurer
5. Report of the Auditors
6. Budget 2004
7. Swiss SNS participation (SNS-presentation, scientific case)
8. News from the European Neutron Scattering Association, ENSA
9. News from the Institut Laue Langevin, ILL
10. SGN/SSDN Activities 2004
11. Elections (chairman, board members, secretary, revisors,
Swiss representatives at ILL-colleges and ILL scientific council)
12. Miscellaneous

Persistence of cluster-like magnetic excitations in the 3-D ordered phase of α -MnMoO₄

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1. Introduction

Spin clusters have played an important role in the study of exchange interactions between paramagnetic ions for a long time. The interest in them soared when it was discovered that clusters with large ground state spin and negative axial anisotropy exhibit magnetisation hysteresis and slow relaxation of the magnetisation at low temperatures [1]. In most examinations of these so-called single molecule magnets (SMM) intercluster interactions were assumed to be negligibly small. However, intercluster interactions exist, and indeed a recent study has shown the effects of these interactions on the quantum behaviour of SMM in the case of a tetrameric Mn-based SMM coupled antiferromagnetically (AFM) to its nearest neighbour [2, 3].

Furthermore, the remarkable experimental observations of quantum phase transitions [4] and field-induced 3-D ordering in weakly coupled AFM dimers [5, 6] or Haldane chain systems [7] were found to originate in a complex interplay of intra and inter-dimer interactions.

Inelastic neutron scattering (INS) has proven to be of essential importance in all these studies, as it allows the direct spectroscopic determination of exchange [5, 6] and anisotropy splittings [8].

We present an INS and magnetic susceptibility study on the tetramer-based Mn²⁺ compound α -MnMoO₄, with three-dimensional (3-D) AFM order below $T_N = 10.7$ K [9]. We report cluster excitations in the ordered phase of α -MnMoO₄, an unprecedented case of molecular magnetic behaviour in a 3-D AFM lattice.

2. Structure

α -MnMoO₄ crystallizes in the monoclinic space group C2/m. It consists of edge-sharing MnO₆ octahedra, which form tetrameric clusters (see Fig. 1) [10]. Along the edges of the cluster the Mn-Mn distance is 3.417 Å and across the short diagonal it is 3.692 Å. The angles at the bridging oxygen atoms vary between 95.73° and 104.13°. The connection between the Mn₄ clusters is made by MoO₄ tetrahedra.

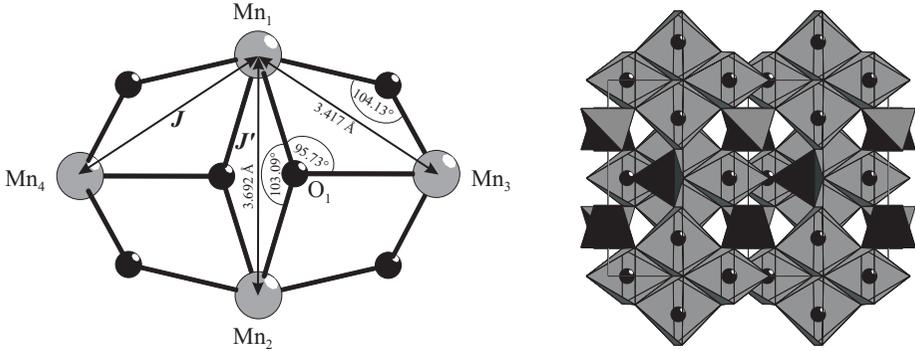


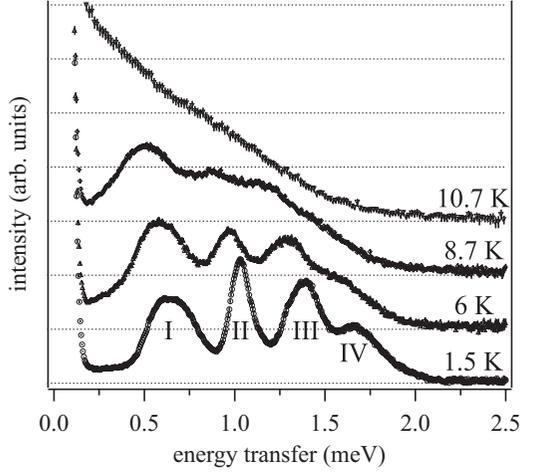
Figure 1: Structure of the Mn₄ cluster with the intermediate oxygen atoms and the relevant distances and angles indicated (left) and the structure of the lattice viewed along the crystallographic *a* axis (right). *J* and *J'* are the exchange parameters along the edges and the short diagonal of the rhombus, respectively.

3. Results

Figure 2 shows the INS spectra of polycrystalline α -MnMoO₄ for $\lambda = 4.75$ Å between 1.5 K and 10.7 K obtained on the time-of-flight spectrometer FOCUS at the spallation neutron source SINQ, PSI Villigen, Switzerland. At 1.5 K well-defined inelastic peaks or bands with varying widths and labelled I to IV are observed. The shapes and widths of the bands are very different, with widths up to three times larger than the instrumental resolution. With increasing temperature the bands become broader and shift to lower energies. The individual bands are no longer resolved and merge into a broad shoulder on the elastic line above approximately 10 K.

The product of the magnetic susceptibility and the temperature χT as a function of temperature decreases from a value of $\chi T = 16.9$ emu K mol⁻¹ at 300 K to $\chi T = 0.5$ emu K mol⁻¹ at 2 K (see Fig. 3). The inset of Fig. 3 shows the low temperature part of χ vs. *T* with a sharp maximum at 10.7 K.

Figure 2: INS spectra of polycrystalline α - MnMoO_4 measured on the time-of-flight instrument FOCUS at SINQ at four temperatures. $\lambda = 4.75 \text{ \AA}$, sum of all scattering angles. The inelastic features I to IV are discussed in the text.



4. Analysis

There are two dominant exchange pathways within the cluster, J along the edges and J' across the short diagonal of the Mn_4 rhombus (see Fig. 1). In terms of these two parameters and with the intercluster interaction treated as an internal field, we obtain the following energy eigenvalues:

$$E(S_{12}, S_{12}, S, M_s) = -J[S(S+1) - S_{12}(S_{12}+1) - S_{12}(S_{12}+1)] - J'[S_{12}(S_{12}+1) - S_i(S_i+1)] - g\mu_B H_{\text{int}} . \quad (1)$$

For the calculation we coupled the spins as follows: $\overset{\uparrow}{S}_{12} = \overset{\uparrow}{S}_1 + \overset{\uparrow}{S}_2$, $\overset{\uparrow}{S}_{34} = \overset{\uparrow}{S}_3 + \overset{\uparrow}{S}_4$, $\overset{\uparrow}{S} = \overset{\uparrow}{S}_{12} + \overset{\uparrow}{S}_{34}$. Powder neutron diffraction measurements revealed a magnetic structure with the four $S_i = 5/2 \text{ Mn}^{2+}$ spins within one cluster aligned parallel, and AFM order of the cluster spins on the two sublattices [9]. There are eight near-neighbour clusters belonging to the opposing spin sublattice. From the parallel alignment of the spins within the cluster, we concluded that J in eq. 1 must be dominant and ferromagnetic (FM). The weaker exchange interaction J' can be either FM or AFM. We expect J' to be negative, because of the relatively large $\text{Mn}_1\text{-O}_1\text{-Mn}_2$ bridging angle of 103° for this pathway. In this case the lowest cluster states, with increasing energy, are given as follows:

$$\begin{aligned} |0\rangle: E(5,5,10,10) &= -50J - 12.5J' - 10g\mu_B H_{\text{int}} \\ |1\rangle: E(5,5,10,9) &= -50J - 12.5J' - 9g\mu_B H_{\text{int}} \\ |2\rangle: E(4,5,9,9) &= -40J - 2.5J' - 9g\mu_B H_{\text{int}} \\ |3\rangle: E(5,4,9,9) &= -40J - 12.5J' - 9g\mu_B H_{\text{int}} \\ |4\rangle: E(5,5,9,9) &= -30J - 12.5J' - 9g\mu_B H_{\text{int}} \end{aligned} \quad (2)$$

We assign the four bands I, II, III and IV in Fig. 2 to transitions from the ground state $|0\rangle$ in eqs. 2 to the four excited states $|1\rangle$, $|2\rangle$, $|3\rangle$ and $|4\rangle$, respectively. With a least-squares fit to the experimental transition energies we obtain the following parameter values: $J = 0.051 \pm 0.004$ meV, $J' = -0.019 \pm 0.003$ meV and $g\mu_B H_{\text{int}} = 0.72 \pm 0.04$ meV.

We used the INS cross-section for tetrameric clusters derived by Güdel et al. [11] to calculate the relative intensities. The experimental and calculated energies and intensities are compared in Table I.

Table I: Experimental and calculated INS excitation energies (eqs. 2) and relative intensities. The cluster ground state is $|5,5,10,10\rangle$. Parameter values: $J = 0.051$ meV, $J' = -0.019$ meV, $g\mu_B H_{\text{int}} = 0.72$ meV.

Band	excited state	E_{obs} (meV)	E_{calc} (meV)	I_{obs}	I_{calc}
I	5 5 10 9	0.65 ± 0.04	0.72	1.00 ± 0.02	1.00
II	4 5 9 9	1.04 ± 0.03	1.04	0.63 ± 0.02	0.62
III	5 4 9 9	1.36 ± 0.05	1.23	0.81 ± 0.08	0.65
IV	5 5 9 9	1.68 ± 0.10	1.74	0.61 ± 0.10	0.69

Taking the spin of each cluster as a *macrospin*, the internal field can be expressed as follows:

$$g\mu_B H_{\text{int}} = 2 \langle \check{S}_{\text{cluster}}^{\nu} \rangle z J_{\text{int}} \quad (3)$$

where $\langle \check{S}_{\text{cluster}}^{\nu} \rangle = 10$, J_{int} is the near-neighbour intercluster parameter, and $z = 8$ is the number of neighbours on the opposite sublattice. We derive a value $J_{\text{int}} = -4.5 \times 10^{-3}$ meV for this AFM parameter, which is about an order of magnitude smaller than the intracluster parameters, in good agreement with the structure.

The parameters obtained from INS were used to calculate the magnetic susceptibility. The dashed line in Figure 3 was obtained by including only the intracluster parameters in the calculation. It shows an increase with decreasing temperature, typical for a FM coupled cluster. Incorporating the intercluster coupling into the calculation leads to the full line in Figure 3, a good reproduction of the experimental data with no adjustable parameter. The sharp maximum in χ at 10.7 K indicates the transition to 3-D AFM order [9].

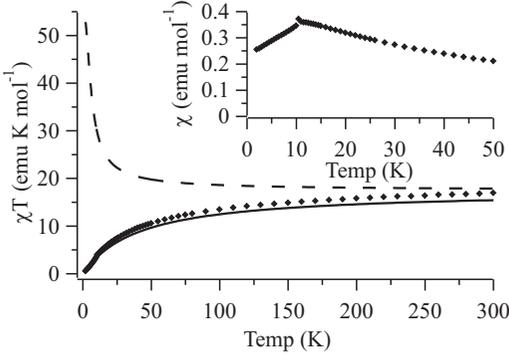


Figure 3: Magnetic susceptibility represented as χT versus T . Dots: experimental points. Dashed line: calculated for isolated Mn_4 clusters with $J = 0.051$ meV, $J' = -0.019$ meV and $g = 2.0$. Full line: including intercluster interactions with $J_{\text{int}} = -4.5 \times 10^{-3}$ meV. The inset shows χ versus T data below 50 K.

5. Discussion

The different widths and shapes of the INS bands are due to the dispersive character of the transition, which is not included in our model. Dispersion effects are also responsible for the discrepancies of calculated and experimental energies and intensities (see Table I). Nonetheless, considering the simplicity of our model, the agreement is good.

The calculated magnetic susceptibility matches the experimental data extremely well. Even above T_N it is dominated by the AFM intercluster interactions, although these interactions are much weaker than the intracuster interactions. We ascribe this to the large number ($z = 8$) of AFM coupled near-neighbour clusters and to the presence of AFM intracuster coupling across the short diagonal of the Mn_4 rhombus.

The FM nature of the dominant interaction parameter J along the edges of the rhombus is extraordinary. In most insulating Mn^{2+} and high spin Fe^{3+} compounds nearest neighbour superexchange is AFM. The net value of J between two Mn^{2+} ions is composed of $5 \times 5 = 25$ orbital contributions, some of which are FM and others AFM. The balance can tip towards a FM net J when the bridging angles ϕ at the ligands approach 90° [12]. We ascribe the FM coupling in the Mn_4 clusters of the title compound to the particular bonding situation at the oxygen atom labelled O_1 in Fig. 1. We note a particularly small angle of 95.7° at O_1 for the pathway J , and this is the dominant FM interaction within the cluster.

6. Acknowledgements

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References

- [1] D. Gatteschi and R. Sessoli, *Angew. Chem. Int. Ed.* **42**, 268 (2002).
- [2] W. Wernsdorfer et al., *Phys. Rev. Lett.* **89**, 197201 (2002).
- [3] B. Barbara, *Nature* **421**, 32 (2003).
- [4] S. Sachdev, *Quantum Phase Transitions*, Cambridge University Press (1999).
- [5] N. Cavadini et al., *Phys. Rev. B* **65**, 132415 (2002).
- [6] C. Rüegg et al., *Nature* **423**, 62 (2003).
- [7] Y. Chen et al., *Phys. Rev. Lett.* **86**, 1618 (2001).
- [8] I. Mirebeau., *Phys. Rev. Lett.* **83**, 628 (1999).
- [9] J. P. Attfield, *J. Phys.: Condens. Matter* **2**, 6999 (1990).
- [10] S. C. Abrahams and J. M. Reddy, *J. Chem. Phys.* **43**, 2533 (1965).
- [11] H. U. Güdel, U. Hauser, and A. Furrer, *Inorg. Chem.* **18**, 2730 (1979).
- [12] R. Schenker, H. Weihe, and H. U. Güdel, *Inorg. Chem.* **40**, 4319 (2001).

Short note on the new time-resolved and polarization option for the SANS-I instrument at SINQ

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Introduction

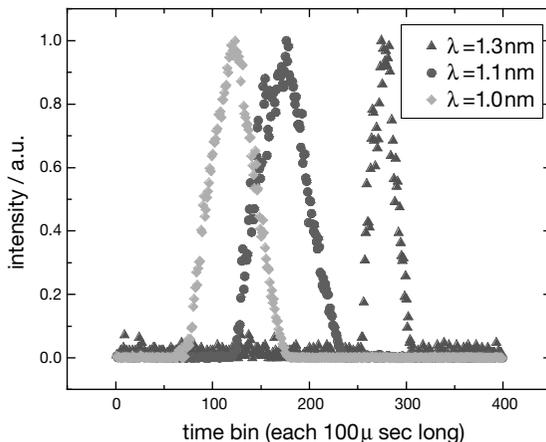
The SANS-I instrument at the Swiss Neutron Spallation Source SINQ is running in user operation since 1998. Recently the instrument has been upgraded with new time-resolved detector electronics and with the option for incident neutron beam polarization. The time-resolved option opens up a completely new field of fast real-time kinetic measurements for the instrument. The polarization option as a second renewal is a very powerful tool for investigations of magnetic nanostructures [2,3], but also a prerequisite for contrast enhancement by exploiting the spin dependent scattering length of hydrogen [4-9].

Time-resolved option

The implementation of the time-resolved option enables to detect structural changes in the range of milliseconds. The new electronics itself would allow to measure down to 1.5 μs time resolution. However, the time resolution is not limited by the electronics but mainly by the velocity of the neutrons and their wavelength spread. For a typical instrument set-up of 10 \AA wavelength and 10 m sample to detector distance the scattered neutrons need already 25 ms to arrive at the detector. This time can only partly be corrected as due to the wavelength spread of typically $\Delta\lambda/\lambda = 0.1$ the fastest scattered neutrons arrive in the above geometry 5 ms earlier on the detector than the slowest. This means that the electronic time resolution of 1.5 μs is sufficiently short for all practical applications. The flexible design of the electronics allows to store up to 4096 frames. The number of time bins and the time width of each single bin can be chosen flexibly. Two different modes of operation are available depending on the sample environment. Either simply a trigger signal is supplied to restart the data acquisition cycle or, in case the readjustment of the initial condition is complex also a slightly more advanced communication between sample environment and electronics is implemented.

To perform experiments down to the millisecond range the dynamic process under investigation has to be repeatable for collecting reasonable statistic for each time frame. Therefore either the dynamic process must be reversible such that one is able to restore the initial condition or in case of irreversible processes enough sample material is required to repeat the experiment many times. An example for the latter type of experiment is a stopped flow experiment. In a stopped flow experiment two or more liquids are mixed rapidly within about 100 ms to investigate fast real-time kinetics like early stages of micelle-to-vesicle transitions. The simplest experiment to test the time-resolved electronics is to record the known wavelength spread of the velocity selector of the instrument by the time-of-flight method. Therefore simply a chopper was placed at the sample position to cut the continuous neutron flux into short time bunches. Then the time dependent intensity at the detector was measured. The results in Fig. 1 show the expected triangular shape of the time pattern for the neutron intensity.

Fig. 1: To test the new stroboscopic mode of the SANS electronics a time of flight experiment has been performed, which measures the wavelength distribution of the neutrons transmitted by the velocity selector.



Polarization option

As a second new option a transmission polarizer has been installed on SANS-I during the 2003 shut down of the accelerator.

An incident polarized beam is a powerful and complementary tool to investigate samples with combined magnetization and density or compositional fluctuations compared to conventional SANS. The polarization has a strong influence on the relative contrast between nuclear and magnetic scattering contributions. This technique has already been successfully applied in other fields, e.g. in the evaluation of magnetization, density and composition profiles at interfaces and surfaces of magnetic nanocrystalline

materials [2]. Other fields of application are biology and polymer chemistry where by dynamic nuclear polarization a contrast on hydrogeneous sample is created by exploiting the strong spin dependent nuclear scattering of protons [4-9]. A polarization option has already been installed, e.g. at the V4-SANS instrument at HMI/Berlin, at the SANS-I instrument at the GKSS-Geesthacht [10], at one of the SANS instruments at NIST and at PAPOL at LLB/Saclay [11]. At PSI we have installed a polarization option similar to that one at HMI [2], as both instruments are very similar in their design (Fig. 2).

Experimental set-up

The incident polarized beam is produced by a supermirror, which may be considered as a device, which has zero reflectivity for antiparallel neutron spin state (-) and total reflectivity for parallel neutron spin state (+). In Fig. 4 the transmission of a Fe/Si supermirror for (+) and (-) neutrons is shown.

At our SANS-I we are using the transmitted (-) polarized beam such that the geometry of the instrument remains unchanged. The polarizer is best placed far away from the sample to suppress parasitic scattering from the polarizer itself. On the remaining flight path between polarizer and sample (15m) it is necessary to apply a small magnetic field of about 10-20 Gauss to preserve the neutron polarization. This small field can easily be achieved by iron plates, which are magnetized by FeNdB permanent magnets (Fig. 2,3). A device for reversing the polarization (spin flipper) will be mounted soon about 1.5 m in front of the sample inside a magnetic shielding box.

Tests on the polarizer have shown a very good transmission of the polarizer of about 42% for 0.5 nm neutron wavelength compared to the unpolarized beam (Fig. 5). The polarization of the beam has been measured with a polarized proton target. By changing the polarization of the proton target the incoherent scattering is changed and thereby its transmission [14,15]. The thickness of the proton target was chosen to have an analysing power of about 0.97. The advantage of this kind of opaque spin filter is that it is not sensitive to the beam divergence, in contrast to a supermirror. The neutron polarization at SANS-I has been measured for several collimation lengths and wavelengths and is shown in Fig. 6.



Fig. 2: Schematic set-up of the polarization option



Fig. 3: a) Adjustment of the polarizer in the collimator segment. b) collimator system with guiding field

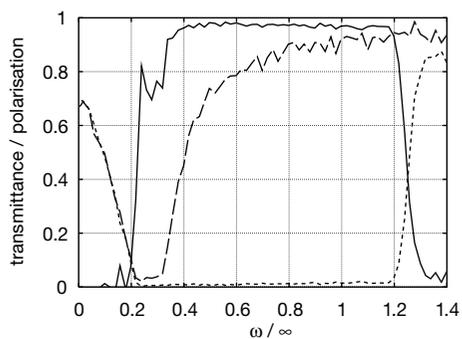


Fig. 4: Transmission and polarization of a Fe/Si supermirror on Si as used for the SANS-I polarizer. The dashed/dotted line is the transmittance for spin up/down neutrons and the solid line is the polarizing efficiency (97% to 98% in the range $0.4^\circ < \omega < 1.2^\circ$ for a wavelength of $\lambda = 4.76 \text{ \AA}$).

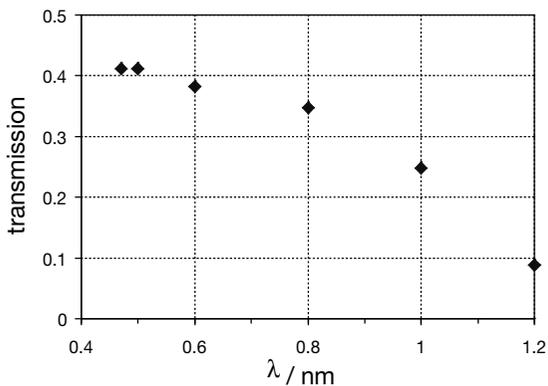


Fig. 5: Transmission of the polarizer $T = I(\text{polarizer in}) / I(\text{polarizer out})$

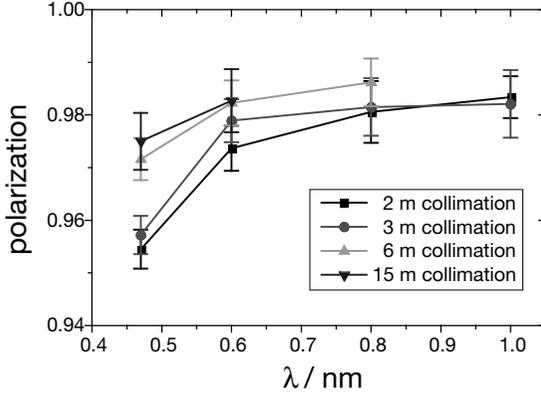


Fig. 6: Neutron polarization for different collimations measured with a polarized proton target.

Applications

Polarized neutrons in SANS are a very powerful tool to investigate magnetic nanostructures. In such experiments a magnetic field is applied to the sample, which defines the polarization direction for both the incident and scattered neutrons. A conventional polarization analysis experiment can separate four partial cross-sections (+ +), (+ -), (- -), and (- +), which connect the neutron spin states (+: parallel, -: antiparallel) before and after the scattering [12]. When no polarization analysis of the scattered neutrons is done (polarization analysis is not foreseen in the present set-up), the intensity at the detector contains both non-spin-flip and spin-flip contributions, and depends on the polarization state of the incident neutrons relative to the magnetisation direction of the sample. In the case when the magnetic moments in the sample are aligned parallel to the magnetic field \mathbf{H} applied perpendicular to the beam direction, the scattering intensity can be written for the two polarization states (parallel and antiparallel) as

$$I^{\pm}(\mathbf{Q}, \alpha) = F_N^2(\mathbf{Q}) + \{F_M^2(\mathbf{Q}) m^2 F_N(\mathbf{Q}) F_M(\mathbf{Q})\} \sin^2 \alpha, \quad (1)$$

where α is the azimuth angle between \mathbf{H} and \mathbf{Q} . The polarization dependent cross-term $m^2 F_N(\mathbf{Q}) F_M(\mathbf{Q}) \sin^2 \alpha$ allows a contrast variation analysis to study magnetization, density and composition profiles at interfaces and surfaces in more detail [2]. If one combines magnetic contrast variation together with a H/D variation of the carrier liquid contrast for example in ferrofluids one is very sensitive for the structural models and is able to identify different magnetic and non-magnetic nanosized components.

Another application of polarized neutrons in SANS is the spin contrast variation technique [12] which is based on spin dependent neutron scattering. The neutron scattering length can be expressed as spin dependent and spin independent parts:

$$b = b_o + b_I \mathbf{I} \cdot \mathbf{s} \quad (2)$$

where \mathbf{I} and \mathbf{s} represent the spins of the nucleus and of the neutron. One of the isotopes with the strongest spin dependent scattering amplitude is ^1H with $b_0 = -0.37 \times 10^{-12}$ cm and $b_1 = -5.84 \times 10^{-12}$ cm. The effect of spin-dependent scattering of its isotope deuterium ^2H is much less profound ($b_0 = -0.667 \times 10^{-12}$ cm and $b_1 = -0.56 \times 10^{-12}$ cm) and the influence from other elements with non-zero spin like ^{13}C and ^{14}N is negligible. The technical challenge on the spin contrast variation is the polarization of the nuclei. To polarize the nuclei in organic material, the only effective way is the dynamic nuclear polarization.

Example: Dynamics of nuclear spin polarization

A first successful experiment using both new devices, the polarization and the time-resolved option, has been performed recently for the investigations of dynamic nuclear polarization (DNP) of proton spins.

DNP creates contrast in SANS due to the strong spin dependence of neutron scattering at protons [4-6]. The electron–nuclear dipolar interaction results in a transfer of the thermal equilibrium polarization of paramagnetic centres distributed in a sample to the nearby nuclei by microwave irradiation close to the EPR line. The nuclei close to the centres are polarized first while far-away (bulk) nuclei reach equilibrium conditions through spin diffusion due to the rapid fall-off of the direct interaction [16]. As the two distinct processes proceed with different time constants, polarization gradients exist around the paramagnetic centres for $t < t_{diff}$ (i.e. for typically a few seconds). They produce a contrast, which can be detected by neutron scattering [9].

Simultaneously time-resolved small-angle polarized neutron scattering (SAPNS) and NMR has been applied, a combination that is a unique tool to study the nuclear polarization build-up around paramagnetic centres during DNP. These experiments for the first time visualise the nuclear polarization process on a microscopic scale. Our model system samples have been glassy slabs of frozen glycerol-water mixtures (deuterated between 88% and 98%), doped with EHBA-Cr^V paramagnetic centres. In those samples each unpaired electron is surrounded by 20 ^1H atoms (the so-called ‘close protons’), embedded in a matrix with a chosen concentration of ^1H atoms (giving the ‘bulk protons’). The bulk protons are observed by NMR. With SAPNS all protons are observed in principle. However, due to the low bulk proton concentration in the chosen samples mainly the close proton polarization influences SAPNS. We have observed that microwave irradiation in a few seconds establishes a large polarization of the close protons. A polarization gradient between the close protons and the bulk protons exists for a short time until spin diffusion equalises the polarization throughout the sample. Figure 7 shows first preliminary results on the time-dependent SANS intensity from a sample of 98% deuterated solution containing protiated EHBA Cr^V complexes. The data has been taken in a stroboscopic experiment with a time resolution of 0.1 sec.

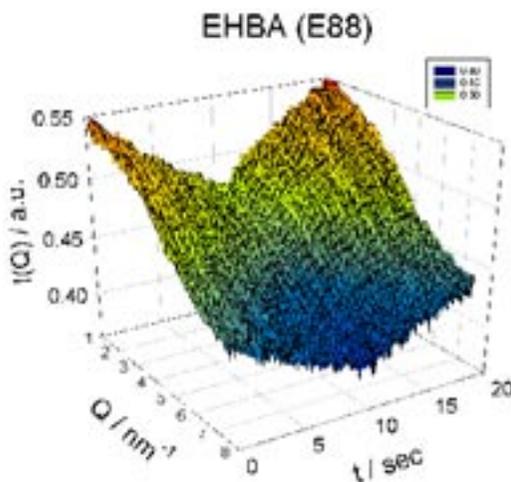


Fig. 7: Time-dependent neutron scattering intensity from a sample of 88% deuterated solution containing 5×10^{19} protiated CrV complexes/cm³ (400 time frames each 50 ms long)

- [1] J. Kohlbrecher, W. Wagner, *J. Appl. Cryst.*, **33**, 804-806 (2000)
- [2] A. Wiedenmann, *J. Appl. Cryst.*, **33**, 428-432 (2000)
- [3] A. Heinemann, A. Wiedenmann, *J. Appl. Cryst.*, **36**, 845-849 (2003)
- [4] W. Knope et al., *J. Appl. Cryst.* **22**, (1989), 352
- [5] R. Willumeit et al., *J. Mol. Struct.* **383**, (1996), 201
- [6] M.G.D. van der Grinten et al., *Neutron News* **6**, (1995), 18
- [7] B. van den Brandt et al., *Europhys. Lett.* **59** (2002) 62-67
- [8] J.B. Hayter et al., *Phys. Rev. Lett.*, **33** (1974) 696
- [9] H.B. Stuhrmann et al., *J. Appl. Cryst.*, **30** (1997) 839
- [10] J. Zhao et al., *Nucl. Instr. and Meth. A* **356** (1995) 134
- [11] H. Glättli et al., *Physica B* **213&214** (1995) 887
- [12] J.B. Hayter, *J. Appl. Cryst.*, **21** (1988) 737
- [13] A. Hoell et al., *JMMM* **252** (2002) 92
- [14] O. Zimmer et al., *Phys. Let. B* **455** (1999) 62
- [15] O. Zimmer et al., *Nuc. Instr. Meth. in Phys. Res. A* **440** (2000) 764
- [16] A. Abragam, M. Goldman, *Nuclear Magnetism, Order*



Neutrons and Systèmes Désordonnés

H.E. Fischer, H. Schober, Éd.s.

L'évolution des thématiques en matière condensée requiert la connaissance conjointe de la structure et de la dynamique de milieux aussi divers que les liquides, les solutions, les verres, les cristaux plastiques, les polymères, les assemblages supramoléculaires, réunis sous le terme de «systèmes désordonnés». La complexité structurale et l'interdépendance des phénomènes dynamiques prévalant dans ces systèmes impliquent des échelles de distance et de temps très étendues, dont l'étude expérimentale préconise une pluralité de techniques expérimentales. Un des objectifs de cette école était de ce fait de préciser les domaines de pertinence des différentes techniques neutroniques disponibles en complémentarité avec d'autres approches instrumentales (diffraction des rayons X, EXAFS, RMN, etc.). Enfin, la confrontation avec les résultats obtenus par simulation et modélisation numériques est essentielle à la compréhension des processus élémentaires dans ces systèmes complexes.

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Neutrons et Matériaux

W. Paulus, J. Meinel, Éd.s.

Les cours présentés dans cet ouvrage ont été développés lors de l'école thématique "Neutrons et Matériaux" au cours de la 10ème édition des "Journées de la diffusion Neutronique" organisée par la SFN (Société Française de la Neutronique) à Trégastel du 16 au 18 mai 2001 en Bretagne. Cette école a proposé aux non-spécialistes du domaine neutronique un large spectre de cours mettant en valeur la diversité des applications de la diffusion neutronique dans divers domaines de recherche, chimie et physique des matériaux, mais aussi sciences de la terre ainsi que sciences pour l'ingénieur. Les cours, donnés par des experts de chaque discipline, couvrent la production de neutrons, les divers mécanismes d'interaction neutron-matière ainsi que l'instrumentation nécessaire. Ils montrent également la complémentarité de la diffusion des neutrons et des rayons X (y compris rayonnement synchrotron), en s'appuyant sur les tous derniers résultats obtenus dans chaque discipline. Cet ouvrage s'adresse donc non-seulement aux enseignants, chercheurs ou étudiants, mais aussi aux industriels, qui souhaitent s'initier à l'utilisation des neutrons.

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Neutrons and Magnétisme

C. Fermon, F. Tasset, Éd.s.

Cet ouvrage est issu des cours donnés à l'école magnétisme et neutrons réalisée dans le cadre des journées de la diffusion neutronique 2000. Ces dernières années, l'étude du magnétisme a connu un renouveau important avec l'apparition de composés présentant des propriétés originales comme les composés à magnétorésistance colossale ou les échelles de spin. La nanophysique n'a pas non plus épargné ce domaine de la physique avec la fabrication et l'étude, d'abord de couches minces magnétiques, puis de petits objets fabriqués dans ces couches avec comme toile de fond l'électronique de spin. Le neutron est, grâce à son moment magnétique, une sonde irremplaçable pour l'étude des configurations magnétiques de solides. Son énergie lui permet aussi d'être très sensible aux excitations magnétiques. Nous avons donc construit le cours et l'ouvrage autour de trois thèmes scientifiques qui illustrent bien l'apport et l'intérêt du neutron pour l'étude du magnétisme : les couches minces et les petits objets magnétiques, la diffraction pour l'étude des poudres et des monocristaux et enfin les excitations magnétiques.

Volume 89 • 2001 • 2-86883-567-8 • 67 €



Diffusion Quasiélastique des Neutrons

M. Bée, Éd.

La diffusion quasi-élastique incohérente des neutrons lents a largement montré ses possibilités d'étude de la dynamique des molécules et des atomes dans les phases condensées. Les énergies mises en jeu sont comparables à celles des barrières de vibration et de rotation des molécules et les longueurs d'onde sont de l'ordre des distances interatomiques. Aussi, tant en physique qu'en chimie ou en biologie cette technique expérimentale est capable de fournir des informations sur les échelles de temps et de distance des phénomènes mis en jeu. Ce cours est une introduction destinée à ceux qui veulent s'initier à cette technique et à ceux qui travaillent dans des domaines voisins comme la résonance magnétique nucléaire. La biologie montre actuellement un grand intérêt pour cette technique. En dépit de la complexité des problèmes posés, la diffusion quasi-élastique se révèle utile dans l'étude de la fonctionnalité des protéines.

Volume 70 • 2000 • 2-86883-436-1 • 45 €



Diffusion de Neutrons aux Petits Angles

J.P. Cotton, F. Nallet, Éd.s.

La diffusion de neutrons aux petits angles (DNPA) est une technique expérimentale qui permet d'étudier la structure de la matière condensée à une échelle de distance comprise entre 1 et 50 nm. Très analogue à la diffusion de rayons X aux petits angles, elle s'est beaucoup développée depuis les années 1970, en particulier en raison de sa remarquable sensibilité à la substitution isotopique. En effet, cette propriété fait de la DNPA une méthode de marquage sans équivalent qui est beaucoup utilisée en remplaçant les atomes d'hydrogène par ceux de deutérium. Elle a aujourd'hui de multiples applications dans la détermination des nanostructures dans le domaine des matériaux polymères, des colloïdes et des composites ainsi qu'en métallurgie. Sa sensibilité aux moments magnétiques des atomes la rend également irremplaçable dans le domaine du magnétisme.

Volume 60 • 1999 • 2-86883-391-8 • 45 €



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Announcements

New SGN/SSDN Members

The Swiss Neutron Scattering Society welcomes the following new member:

- K. Mortensen (Danish Polymer Centre, Risø National Laboratory, DK)

Presently the SGN has 189 members.

SINQ Users' Meeting 2004

The 6th SINQ users meeting will be organized at PSI on Thursday, 22/01/2004. The focus of the meeting is on the presentation of the results obtained by the various user groups at SINQ. It should also enhance the discussion among the user community and the responsables at the Swiss neutron scattering facility. The meeting will consist of scientific oral and poster sessions. Recent upgrades and news on the SINQ instruments will be presented as well as actual information about the user program. For more detailed information please have look at the meeting's webpage:

http://sinq.web.psi.ch/sinq/usmeet_6/meet6.html

Open Positions at ILL

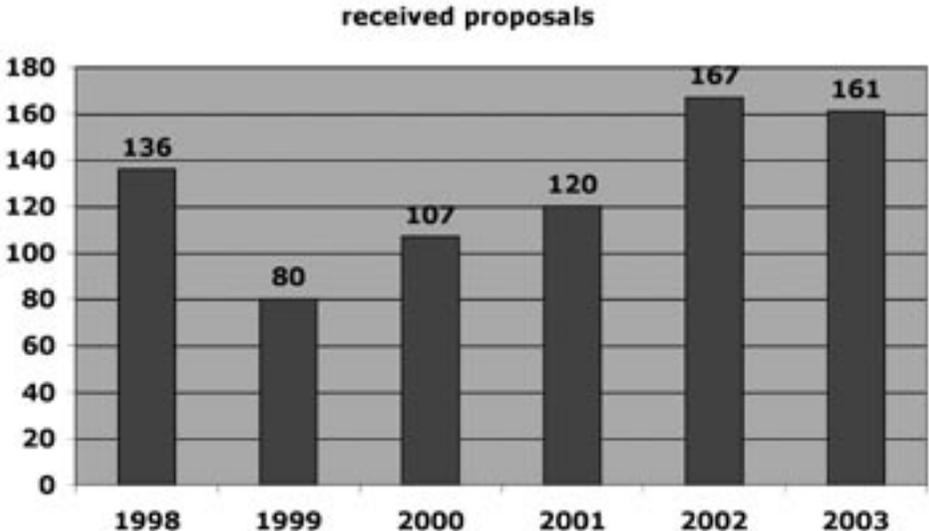
The 'Swiss Bundesamt für Bildung und Wissenschaft, BBW' regularly informs us about open positions for scientists, engineers or technicians at the Institut Laue Langevin (ILL), Grenoble. Quite often the deadline for the application has already passed before the next issue of 'Swiss Neutron News' is published such that an announcement of the open job here does not make sense anymore.

Therefore we would like to bring to your notice that you can easily check the actual open positions at ILL at the ILL-homepage: <http://www.ill.fr> following the link 'Job Offers'.

News from SINQ

Stefan Janssen, SINQ Scientific Coordination Office, Paul Scherrer Institut

The last months of the year 2003 have been very exciting and encouraging for SINQ. First we learned that our 'Access Proposal' within the 'Integrated Initiative of Neutron and Muon sources, NMI3' of the EU framework program 6 was evaluated successfully and very positively. The program will start on 01/03/2004 and will give us the opportunity also in the future to support our users from EU countries and associated states as we have already been doing since 2002.



Furthermore, we received an overwhelming number – namely 102 – of new proposals in November 2003 (which clearly exceeds the existing record of 89 proposals in I/03). 21% out of those are longterm proposals, the others ask for beamtime in the upcoming SINQ cycle between May and August 2004. 66% of the proposals have been submitted from outside Switzerland and 42% are eligible within the 'EU Access Program'. The strongest scientific topics among the new proposals are 'Materials Science' (22%), Magnetism (21%) and Soft Condensed Matter (17%).

In 2004 the extended guide hall (see cover page of this SNN issue and contribution in the previous issue, Nr 23) with plenty of space for the users (laboratories, computing facilities) will be made available. It will host the new SINQ backscattering spectrometer MARS which is well on its way as well as the new thermal triple-axis spectrometer TNT. Both instruments are expected to be commissioned in 2005. Earlier, namely in fall 2004, the new 15 Tesla magnet will be available for experiments (first on RITA-II) which will open a vast field of new experimental possibilities at SINQ.

Presently the annual shutdown of the proton accelerator enables us to inspect and upgrade the instruments and sample environment devices. Also the neutron guide for the MARS spectrometer is being prolonged. After that shutdown – in May 2004 – we look very much forward to meeting you again at the instruments around SINQ.

Conferences 2004

for an updated list please also have a look at: <http://sinq.web.psi.ch/sinq/links.html>

date	place	conference
09–16/01	Los Alamos	LANSCE Neutron Winter School http://lansce.lanl.gov/neutronschool/index.html
13–16/01	Tokyo	Neutron Optics and Detectors http://nop.riken.go.jp/workshop/nop2004/
22/01	Villigen	6 th SINQ Users' Meeting http://sinq.web.psi.ch/sinq/usmeet_6/meet6.html
27–28/01	Lucas Height	0 th Workshop on Instrumentation at Australia's Replacement Reactor http://www.ansto.gov.au/ansto/bragg/workshops/workshop10.html
09–13/02	Benasque, ES	Interplay of Magnetism and Structure in Functional Materials http://www.ecm.ub.es/workshop2004/home.html
09–13/02	Grenoble	14 th ESRF Users Meeting http://www.esrf.fr/Public/Conferences/UsersMeeting2004/
22/02–02/04	Grenoble	HERCULES 2004 http://www.grenoble.cnrs.fr/hercules.html
23–27/02	Hanoi	Dynamics of Disordered Materials on the Nanometer Scale http://www.engconfintl.org/4ah.html
22–26/03	Montreal	2004 March Meeting of the APS http://www.aps.org/meet/MAR04/
30/03–01/04	London	Materials Congress 2003 http://www.iom3.org/congress2004
03–06/05	Knoxville	11 th SNS Beam Instrumentation Workshop http://www.sns.gov/biw04/

date	place	conference
27–30/05	Samarkand	International Symposium on HTSC taylanov@yandex.ru
06–10/06	College Park	2 nd American Conference on Neutron Scattering (ACNS) http://www.ncnr.nist.gov/acns/
27/06–01/07	Seeheim	2 nd Seeheim Conference on Magnetism SCM 2004 http://www.tu-darmstadt.de/magnetism/
05–09/07	Orleans	Networks in Physics and Biology Interactions, http://www.lptl.jussieu.fr/users/mmi/orleans/ anongal.html
26–30/07	Karlsruhe	Int. Conf. on Strongly Correlated Electron Systems (SCES'04) http://www.sces04.uni-karlsruhe.de
24–27/08	Krasnoyarsk	EASTMAG-2004 http://eastmag-2004.kirensky.ru

Third European Conference on Neutron Scattering: ECNS 2003 in Montpellier

Joel Mesot

Laboratory for Neutron Scattering, Paul Scherrer Institute & ETH Zurich

After Interlaken (1996) and Budapest (1999), the third European conference on neutron scattering was held in Montpellier, September 3-6, 2003. It was coupled to the now traditional introductory course that took place in Saclay, September 1-2. During this course most aspects of neutron scattering were presented to more than 40 participants from all over the world. The first day was devoted to the general concepts related to neutron scattering, including fundamental physics with neutrons, and some practical exercises. The second day was dealing on one side with topical aspects like magnetism, biology and materials science, and on the other side with a visit of the “Laboratoire Léon Brioullin (LLB)”. After such a dense program, the whole school could relax in the TGV on his way to Montpellier, host of the ECNS conference that took place in the beautiful conference center: Le Corum.

The conference, with over 700 participants was perfectly organized by the team of Prof. René Vacher (Univ. Montpellier), and the LLB, in collaboration with the Institute Laue Langevin, the French Neutron Society and the European Neutron Scattering Association. During the opening session Prof. R. Cowley was awarded the Walter Hälgl prize. The heart of the conference consisted of 11 subject categories divided in parallel oral sessions, poster presentations and two afternoon panels devoted to the future of neutron scattering in Europe (see also first issue of ‘Neutron News’ in 2004). On the final day, 10 prizes were awarded to the following young scientists: S. Arrese-Igor (Univ. of the Basque Country, Spain), J. Baumert (ILL, FR), P. Bentley (Univ. of Leeds, UK), C. Boullier (CEA-Grenoble, FR), R. Gilardi (ETH Zurich & PSI, CH), A. Guenther (GKSS Geesthacht, DE), O. Majerus (Uni. Paris 6&7, FR), M.C. Rheinstädter (ILL, FR & FZ-Jülich, DE), S. Vivet (Uni. Paris XII, FR), M. Zamponi (FZ-Jülich, DE). Congratulations to all of them from Swiss Neutron News.



Donation of the 'Walter Halg prize' by its founder to Prof Roger Cowley.



The SINQ booth waiting for the first poster session.



The main auditorium of the conference center 'Le Corum' during one of the plenary sessions.



The conference chairman Prof. René Vacher mastered not only a great conference but also his university orchestra since he was acting as conductor during the concert.



RESEARCH PROPOSAL
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SINQ
 Swiss Spallation
 Neutron Source

Experiment Title:	Proposal number (to be completed by SINQ-SCO)
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<input type="checkbox"/> Short term proposal (next allocation period)	<input type="checkbox"/> Long term proposal (2 years)
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Proposer <i>(to whom correspondence will be addressed)</i> Name and first name: Address:	Phone: Fax: Email:
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Co-proposer(s): Name:	Address: <i>(if different from above)</i>	Phone/Fax/Email:
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Sample description		
Substance and formula:	Mass:	Size:
<input type="checkbox"/> Polycrystalline <input type="checkbox"/> Single crystal <input type="checkbox"/> Multilayer <input type="checkbox"/> Liquid		<input type="checkbox"/> Gas
Sample Container:	Space group:	Unit cell: a= b= c=

Area of Research		
<input type="checkbox"/> strongly correlated electron systems	<input type="checkbox"/> quantum spin systems	<input type="checkbox"/> superconductivity
<input type="checkbox"/> structure	<input type="checkbox"/> dynamics	<input type="checkbox"/> magnetism
<input type="checkbox"/> polymer systems	<input type="checkbox"/> colloidal systems	<input type="checkbox"/> materials science
	<input type="checkbox"/> biological systems	<input type="checkbox"/> others

Hazard	
Is there any danger associated with the sample or sample environment? <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> Uncertain If yes or uncertain, please give details of the risks associated:	

Experimental details			
Instrument	Days	Sample cond.: Temp., Pressure, Magn. field	Exp. cond.: E, ΔE, λ, Δλ, Q, ΔQ

<input type="checkbox"/> New SINQ user	<input type="checkbox"/> New proposal	<input type="checkbox"/> Continuation of.....	<input type="checkbox"/> Resubmission of.....
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Requested dates:	Unacceptable dates:

Experiment Title:

Research funded by:

Scientific background/Aim of experiment: *(Please restrict to the space given within this box!)*

I certify that the above details are complete and correct.

Date:

Signature of proposer: