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Address: Sekretariat SGN/SSDN
Laboratory for Neutron Scattering
ETHZ & PSI
5232 Villigen PSI, Switzerland
phone: +41-(0)56 - 310 2087
fax: +41-(0)56 - 310 2939
www: http://sgn.web.psi.ch

Bank Account: 50-70723-6

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On the cover:

Albert Furrer, head of the 'Laboratory for Neutron Scattering' at the ETH Zurich and the Paul Scherrer Institute retired at the end of November 2004. In order to appreciate his outstanding merits in the field of neutron scattering in general and in Switzerland in particular, the Swiss Neutron Scattering society awarded to him the honorary membership (see article in this issue). The cover photo shows the four former ENSA chairmen: Albert together with Fabrizio Barocchi, Dieter Richter and Bob Cywinski on the occasion of his retirement symposium at PSI in October 2004.

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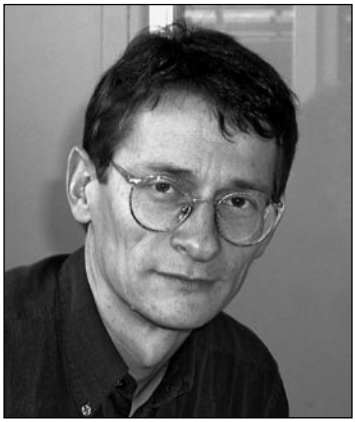
The President's Page



Dear members,

during a symposium in October on the occasion of his retirement and in celebration of all his achievements, Albert Furrer was awarded the honorary membership of our society. You will find two articles in this issue and a picture gallery of the corresponding events. At this point I would like to thank Albert again for all he did as founder of our society, co-founder of ENSA, 'co-father' of SINQ, advocate of neutron scattering, head of LNS, eminent scientist, inspiring teacher and - last but not least - very good friend. Thank you, Albert!

The successful start and the first call for proposals for FRM-II marks a change of perspective for the Swiss neutron users: Switzerland is now 'sandwiched' between two very powerful neutron sources, in the north-east FRM-II and in the south-west ILL; both in immediate vicinity. How will this alter the habits of the users and what will be the impact on our home-source SINQ? The answer to the first question is quite clear: There are now more opportunities to perform excellent experiments in our vicinity and I'm sure that the Swiss community will act accordingly and become even more active. The answer to the second question is not that obvious. Low and medium flux sources are and will undoubtedly be places for education of students, for method developments and exploratory experiments in the future. However, people at PSI will not be satisfied with such a role and an investigation of the past and present clearly demonstrates that SINQ was very successful in a highly competitive environment. This resulted in 11 PRL and 26 higher impact publications (impact factor >2) in 2004, a record value taking into account the raw neutron flux and the number of people and instruments. In addition, the number of proposals was continuously increasing over the last few years and culminated in an all time high of 213 in 2004. I'm positive that SINQ can keep this pace if it will concentrate on its two major assets: Strong in-house research, cutting edge facility and instrument developments (and implementation of these new developments). A prerequisite for this is that the scientists and engineers have the capacity to do research and developments in addition to their operational duties. PSI's NUM-department (condensed matter research with neutrons and muons) is addressing this issue by reorganizing its structure for 2005.

The European Neutron Scattering Association (ENSA; http://neutron.neutron-eu.net/n_ensa) has been occupied with the ESS-project and the NMI3-program in the past years. While its input and collaboration on ESS and NMI3 was essential, there was no real capacity left for activities concerning neutron users. In order to intensify this aspect again and to learn about the neutron user base, its opinion and needs, ENSA has launched a questionnaire (similar to the one almost ten years ago). You will find it on the web:

http://neutron.neutron-eu.net/n_ensa/n_survey

It is extremely important that this questionnaire is answered by as many neutron users as possible in order to have a representative overview and a sound legitimation for future science political statements. Hence, please answer this questionnaire in time (before February 18, 2005).

Concerning a Swiss participation at SNS, we are presently submitting proposals to different funding bodies to develop and manufacture an actively shielded 16T-magnet. This will be the first of its kind for neutron scattering and most likely for quite some time the only larger magnet at SNS, with very high visibility and impact. This contribution will provide the Swiss neutron users an entry for scientific collaborations and a small amount of guaranteed measurement time.

Peter Allenspach

Supramolecules under Stress: a Study of Structural and Magnetic Properties

Thomas Geue
Paul Scherrer Institute, Laboratory of Neutron Scattering,
CH-5232 Villigen PSI, Switzerland

Yves Bodenthin, Ullrich Pietsch, Jörg Grenzer
University Potsdam, Department of Physics, D-14415 Potsdam, Germany

Guntram Schwarz, Dirk Kurth, Helmuth Möhwald
Max Planck Institute of Colloids and Interfaces, D-14424 Potsdam, Germany

Introduction

"There's plenty of room at the bottom!"

The classic talk [1] that Richard Feynman gave on December 29th, 1959 at the annual meeting of the American Physical Society at the California Institute of Technology (Caltech) was a milestone for micro- and nanostructure materials research. Growing demands in science and industry led to micro-technologies, i.e. the challenge to build smaller and smaller structures starting from macroscopic material and reducing the size e.g. by lithography. On the other hand, Feynman initiated the discussions about nano-technology: the challenge to build "bigger" structures from individual molecules or atoms. The concept of supramolecular structures [2] follows this approach to build functional aggregates such as quantum structures, molecular machines, nano-engineered proteins or molecular assemblies.

Consequently, metallo-supramolecular modules (MEMOs) are at the focus of materials research for the construction of functional devices for recognition (sensing), transformation (catalysis), and translocation (signal transduction) [2]. The increasing importance of MEMOs is based on the fact that an assembly of metal ions and ligands provides an elegant and efficient access to a wide variety of well-defined structures and value-adding functions [3]. Metal ions collect and spatially direct the assembly of ligands according to predetermined coordination algorithms. The final properties are tailored through the judicious choice of steric and electronic ligand–metal ion interactions.

The occurrence of semi-occupied d-orbitals gives rise to some of the most prominent properties of MEMOs including strong absorption, high quantum yields, suitable excited state life times, luminescence, and tuneable redox-states. The splitting of the d-orbitals in a ligand field of appropriate symmetry and strength can give rise to thermally or photo-induced spin transition and spin crossover phenomena, the most intriguing ones being light induced excited spin state trapping (LIESST) [4], reverse [5] and low spin LIESST [6], but also metal-to-ligand charge transfer in nitroprusside [7], metal-to-metal charge transfer in prussian blue analogues [8], valence tautomerism [9], as well as ligand driven light-induced spin-state change (LD-LISC) [10].

The conversion between a low-spin (LS) and a high-spin (HS) state is typically observed in transition metal ion compounds with a $3d^n$ ($4 \leq n \leq 7$) electronic configuration, the most extensively studied element being the Fe^{II} ion. In a ligand field of octahedral symmetry, the d-orbitals split in 3 low-lying t_{2g} and 2 high-lying e_g levels. Thermal induced spin transitions occur if the energy separation between the t_{2g} and e_g orbitals is approximately equal to k_BT. In the case of the Fe^{II} ion, the LS state arises form a closed-shell t_{2g}^6 electronic configuration and the HS state from a $t_{2g}^4e_g^2$ electronic configuration, respectively. The spin crossover to the HS state is generally accompanied by a change in optical and magnetic properties, as well as a lengthening of the metal ion–ligand bond due to the occupation of the anti-bonding e_g subset [11].

Two principle strategies have been adopted in ligand design in order to affect the spin state of the coordinating metal ion. The strength of the ligand field can be reduced by steric hindrance in the coordinating ligands, thus, making the HS configuration more favourable [12]. For instance, 2,2':6',2"-terpyridine (tpy) induces a strong ligand field and, therefore, the resulting complexes with iron(II) of the form $[Fe(tpy)_2]X_2$ are exclusively LS, independent from the counter ion X. While substitution in the 4'-position of the central pyridine ring has no effect, it has recently been recognised that bulky substitutents in the 6 and/or 6"-position does affect the spin state.

A macroscopic response function of the system, e. g. the magnetisation as a function of temperature, relies on co-operative effects of the individual active centers. In the solid state, co-operativity results from the fact that the equilibrium geometries of the LS and HS states are different and is, therefore, introduced through the degree of interactions between the active centers. A common approach to achieve tight intersite coupling is based on the formation of coordination polymers through bridging ligands, such as substituted triazoles.

Here, we report a novel approach to affect spin crossover by introducing mechanical strain through an amphiphilic phase transition in a lamellar superstructure containing a quasi one-dimensional rigid-rod type metallo-supramolecular polyelectrolyte (MEPE) based on the ditopic bis-terpyridine 1,4-bis(2,2':6',2''-terpyridine-4'-yl)benzene (Fig. 1).

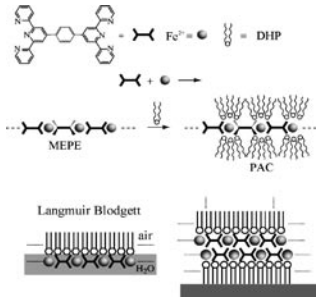


Fig.1: Self-assembly of ditopic bisterpyridine ligands, transition metal ions and amphiphiles results in metallo-supramolecular coordination polyelectrolytes (MEPEs) and the corresponding polyelectrolyte-amphiphile complexes (PACs). Thin films of PAC were prepared by means of Langmuir-Blodgett technique.

MEMO devices possess diverse reactive, kinetic and thermodynamic properties, making them attractive for electronic, magnetic and photonic applications. There are several ways to prepare extended assemblies of metallo-supramolecular devices, including thin films and monolayers on planar [13,14] and colloidal interfaces [15], as well as liquid crystalline phases [16,17]. Langmuir-Blodgett films are ideal systems to investigate on the one hand the interactions between polyelectrolytes and amphiphiles on the macroscopic scale and on the other hand changes in the Fe2+ surrounding and its energetic condition on a microscopic scale.

The investigated system consists of metallo-polyelectrolytes (MEPE), prepared in a aqueous solution by self-assembly of ditopic 1,4-bis(2,2':6',2''-terpyridin-4'-yl)benzene and Fe^{2+} ions [12]. Subsequent self-assembly of MEPE and dihexadecyl phosphate amphiphiles (DHP) results in a completely non-covalent, hydrophobic polyelectrolyte-amphiphile-complex (PAC) [17]. Under these conditions the composition of PAC shows six amphiphiles per repeating unit of MEPE.

As shown recently [17] PAC spreads at the air water interface, and the resulting Langmuir layers can be transferred onto solid supports yielding highly organised anisotropic Langmuir-Blodgett (LB) multilayer films. However, the exact structure of Fe-PAC multilayer films on solid supports has not been addressed so far.

The present study was undertaken to gain detailed insight into the structure of Langmuir-Blodgett films, which is of importance for the understanding of the interactions between MEPE and amphiphiles as well as the principal parameters that determine the physical properties like molecular magnetism [18,19].

The architecture of the LB-films was investigated by energy-dispersive X-ray reflectivity (XRR) and in-plane diffraction [20]. The XRR data of LB-films measured at room temperature reveal Kiessig fringes as well as Bragg peaks (not shown here), confirming the strict stratification of the supramolecular units with an interlayer lattice spacing of (5.6±0.1) nm. Compared to the length of DHP (2.4 nm) this spacing corresponds to the head-to-head or tail-to-tail arrangement, respectively, of two adjacent PAC strata (Y-type arrangement). In addition, a distinct in-plane ordering is observed characterised by the appearance of a single in-plane Bragg peak with an in-plane lattice parameter of (0.42±0.01) nm. This peak is consistent with hexagonal in-plane packing of the alkyl chains of DHP within the strata of the multilayer.

Upon heating, both the in-plane and out-of-plane ordering change indicating a phase transition (Figure 2a). Above 318 K, we observe a change, of the interlayer spacing from 5.6 nm to (5.2±0.1) nm accompanied by a weakening of the Kiessig interference fringe contrast as well as the disappearance of the in-plane Bragg peak. At this temperature, the alkyl chains of DHP start to disorder, which increases the interfacial roughness between the strata and leads to a bending of the structure. Upon cooling, the in-plane Bragg peak and the Kiessig fringes were recovered showing the reversibility of the phase transition. When heated above 338 K the multilayer structure changes irreversibly. The interlayer spacing is reduced to (4.6±0.3) nm, which is accompanied by a complete loss of the Kiessig fringes indicating significant interfacial roughness. Again, no in-plane Bragg peak was observed corresponding to the disappearance of the in-plane ordering. At this point, the supramolecular film is assumed to consist of heavily distorted PACs.

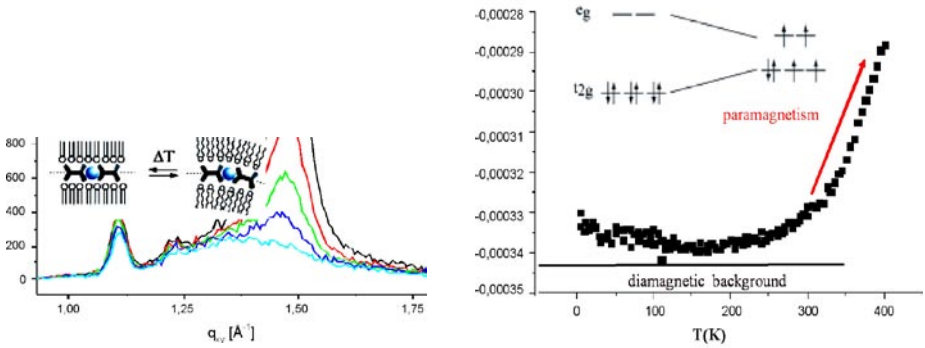


Fig2: Left: temperature resolved grazing incidence diffraction measurements of a PAC Langmuir Blodgett film. The amphiphile phase transition is indicated by the loss of the in-plane diffraction peak at 50°C. Right: SQUID of the temperature induced phase transition in the amphiphilic mesophase is utilised to distort the coordination geometry of the metal centres. Consequently, the energetic separation of the subsets of the orbitals changes giving rise to spin crossover.

To verify this hypothesis we determined the magnetic moments of the sample using SQUID (superconducting quantum interference device) in the temperature range from 5 K to 400 K. Figure 2b shows the temperature dependent magnetic moment for two samples consisting of 11 and 15 Langmuir monolayers, respectively, deposited on silicon wafers. Whereas the material behaves diamagnetic at low temperatures, we observed an increasing paramagnetic signal above room temperature. Even at temperatures above 400 K we did not observe saturation of the paramagnetic signal.

In order to determine the structure of the coordination sphere of the metallo-units, we perform EXAFS (extended X-ray absorption fine structure) at the iron K_α absorption-edge (E = 7.1 keV) [21]. Although the amount of Fe(II) in the sample is small, the

corresponding EXAFS signal is strong enough to extract the next neighbour coordination sphere around the metal center. We noted that the room temperature spectra can only be simulated with a two-shell model assuming two different Fe-N bond distances, R_1= (0.176±0.002) nm and R_2=(0.218±0.002) nm, and occupation numbers of 4 and 2, respectively. These values correspond to a distorted octahedral coordination geometry with 4 N-atoms in the equatorial positions and two in the terminal positions of the distorted octahedron. These determined bond distances are in good agreement with data from single crystal structure analysis of bis-terpyridine iron(II) complexes [22]. Therefore, we conclude that the coordination octahedron is oriented with the long axis parallel to the substrate surface and parallel to the axis of the PACs.

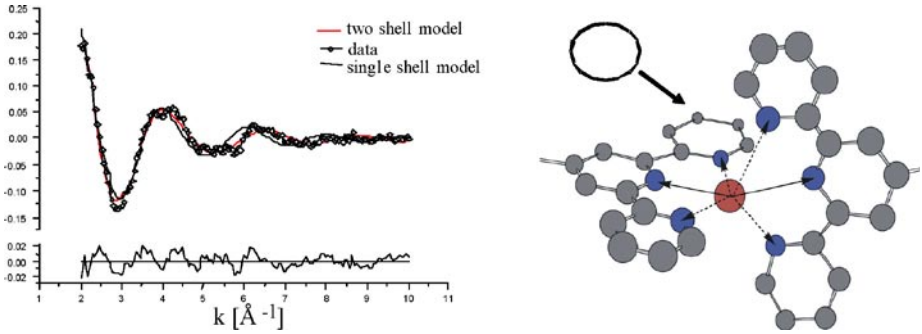


Fig.3: Typical EXAFS function of PAC films. The data can only fitted using a two shell model with iron-nitrogen distances R1 = 0.176 nm and R2 = 0.218 nm and occupation numbers 4 and 2, respectively.

Temperature dependent EXAFS measurements indicate a structural change in the coordination geometry. In terms of the two shell model, the data can be interpreted either by an uniform increase of the octahedron dimensions by 2% or by an uniaxial elongation of the long axis by 4% for increasing temperature up to 348 K. Considering all the data, a temperature rise results in structural changes at all length scales. A change in the coordination geometry (that is the bond length as indicated by EXAFS) is expected to affect the crystal field splitting. In particular, a lengthening of the Fe-N bond length should reduce the splitting of the d-orbital subsets thus opening the way for spin transitions in this material.

Spin resolved neutron reflectivity (SNR) measurements were used to probe the magnetic moment of Fe^{2+} centers at room temperature [23]. Here, the direction of the magnetic moment of the complex is oriented perpendicular to the scattering plane using an external magnetic field of 0.7 T. The scattering plane is defined by the vectors of the incident and reflected waves.

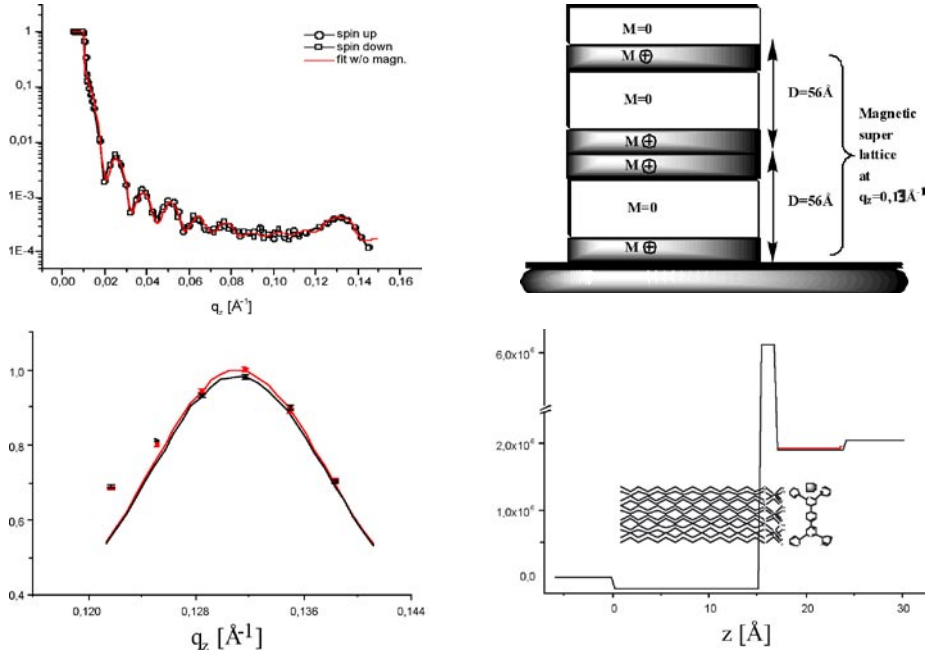


Fig.4: Spin resolved neutron reflectivity curve and difference in Bragg peak intensities for both spin directions. The vertical sequencing and deduced modelling of the films is shown on the right hand side .

The first order Bragg peak appears at 0.13 $Å^{-1}$ and is caused by both the core and magnetic scattering of the atoms. If we assume that the spin of the neutron remains unchanged after interaction with sample (that is a non-spin flip analysis) the scattering intensity is proportional to the scattering length $b = b_{nuc} \pm p \sin\Theta$, where b_{nuc} is the scattering length of the nucleus, *p* the magnetic scattering length, and Θ is the angle between the magnetic moment of the sample μ_s and the scattering plane. The quantity b_{nuc} is independent from the scattering angle and the magnetic moment of the neutron μ_n. Through the external field μ_s is oriented parallel (spin up) or anti-parallel (spin down) to μ_n ($\sin\Theta=1$). As indicated by the equation above, the scattering intensity depends on the orientation of the magnetic moment of the sample with respect to the spin polarisation of the probing neutrons [24]. For the present supramolecular structure we determined a difference in reflected intensities of the first Bragg peak for spin up and spin down neutrons of approx. 2 % at room temperature. Simulation of the reflectivity data yielded *p*, which corresponds to a magnetic moment of (0.6±0.3) μ_B per iron ion, where μ_B is the Bohr magneton. In comparison, Constable et al. [12] reported a

value of 5.3 μ_B over the temperature range 290 to 40 K. We assume that the experimentally determined value represents a lower limit and since saturation has not been achieved the magnetic moment should increase with temperature as more and more Fe-centers become distorted. Measurements at higher temperature are not possible with this method due to the decreasing intensity of the structural Bragg peaks above the phase transition temperature.

Independently, we determined the magnetic moment by X-ray magnetic circular dichroism (XMCD) [25], which offers higher accuracy even for thin film materials compared to SNR. Here, the X-ray reflectivity of the multilayer was measured at a fixed angle of incidence (α_i=2°) using left- and right-handed circular polarised synchrotron radiation at room temperature (308 K) (see Figure 5).

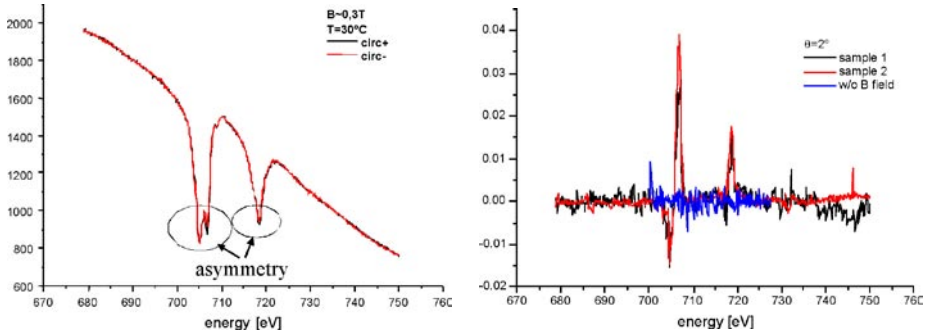


Fig.5: XMCD measurements at the L3,2 edge of iron (left). Right: The asymmetry A(E) = $(I_+ - I_-)/(I_+ + I_-)$ between left- and right circularly polarised light indicates the appearance of molecular magnetism. The blue line indicates A(E) without an applied magnetic field.

Due to the E^{-2} dependence of the reflectivity coefficient the overall reflectivity decreases as a function of energy E of the probing beam. Additionally, there are two minima at about 706 eV and 718 eV corresponding to the L_3 and L_2 absorption edges of iron. Applying an external magnetic field of about B= 0.3 T perpendicular to the direction of the scattering vector and in the scattering plane, the intensities of the minima differ for right (+) or left (-) circularly polarised radiation.

In Figure 5 (see above), the difference in reflectance is displayed by the asymmetry ratio $A(E) = (I_+ - I_-)/(I_+ + I_-)$. The non-zero asymmetry ratio at both absorption edges is a clear evidence of the magnetisation of the sample, which is supported by the control experiment that no dichroic signal is observed without an applied field. Generally, the refractive index n= 1- (δ ± Δδ) + i (β ± Δβ) is a complex quantity and both real (dispersion δ) and imaginary part (proportional to absorption) depend on the electron density and the contributions (Δδ, Δβ) from the magnetic moment of the material [26].

Usually, XMCD is measured in transmission geometry where the absorption term dominates the experiment. This is not the case for the present experiment because in reflection geometry both terms ($\Delta\delta$, $\Delta\beta$) contribute to the signal. To interpret the data, we use ab-initio calculations to evaluate the energy dependent contribution of $\Delta\delta(E)$ and $\Delta\beta(E)$ to the reflectance [27]. These values are used to determine the complex refractive index, which in turn serves to compute the energy dependent reflectance with the Fresnel equations. Applying sum rules to the absorption part $\beta\pm\Delta\beta$ of the complex refractive index n we obtained a magnetic moment of (0.5±0.3) μ_B per iron ion for the spin-momentum and (0.01±0.01) μB per iron ion for the orbit-momentum. These values are in good agreement with the neutron measurements presented before.

To conclude, we demonstrated that a phase transition in an amphiphilic mesophase can induce sufficient mechanical strain to distort the coordination sphere of the tightly coupled Fe(II) centers in MEPE. The distortion is strong enough to reduce the strength of the ligand field, giving rise to spin transition from low to high spin state. The observed high temperature molecular magnetism differs from that of other magnetic materials. Instead of competing spin ordering versus thermal disorder, the presented material is characterised by spin transition induced by gap reduction. This approach is remarkably modular and, therefore, provides extensive control of the spin crossover response function. Through the design of the amphiphiles and the ligands it should be possible to fine-tune the 3 dimensional organisation of the active centers and their interactions. In addition, liquid crystalline materials are readily processed into various device architectures [28].

"Up to now, we have been content to dig in the ground to find minerals. We heat them and we do things on a large scale with them, and we hope to get a pure substance with just so much impurity, and so on. But we must always accept some atomic arrangement that nature gives us. We haven't got anything, ... , with the impurity atoms (or molecules – the authors) exactly arranged 1,000 angstroms apart, or in some other particular pattern." [1]

The introduction of different metal ions, randomly or deliberately, ligands, and amphiphiles presents further options in controlling these functions. Finally, the concept can be extended to virtually all metallo-supramolecular polymers with suitable electronic configurations giving access to a wide variety of new materials.

Acknowledgements

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Monte Carlo Simulations of Neutron Scattering Instruments and Facility Components

G. Zsigmond and U. Filges
Laboratory for Neutron Scattering,
ETH Zürich & PSI Villigen, CH-5232 Villigen PSI, Switzerland

Abstract

Numerical simulations in science become more and more important in building a bridge between theory and experiment. We show here how recent developments of the Monte Carlo software packages, McStas and VITESS, for simulation of neutron scattering instruments allow for the computation of very complex neutronic systems.

1. Why Monte Carlo simulations?

Nowadays, computer hardware, memory and speed are being continuously improved. User friendly open-source MC simulation packages such as VITESS, McStas, etc become more and more easily available. For complex instruments - computer simulations are much faster and more efficient than analytical methods [1].

Moreover, MC simulations describe conditions where analytical approaches are not exact: realistic moderator spectra; optimization of guide and bender systems; large focusing and detector systems with broad solid angles causing non-linearity; non-ideal conditions, as misalignments, waviness, effect of gravity, etc.

We underline that MC simulations complement - do not replace - analytical methods. Analytical approaches mainly describe one-dimensional distributions but reveal relationships that are difficult to understand in numerical simulations. MC simulations easily provide very detailed acceptance-, phase- and other diagrams which enlighten complicated correlations between time, spatial, phase-space and spin coordinates of the neutrons.

In our days, numerical simulations in science become more and more important in building a bridge between theory and experiment. We can envisage that in the near future virtual computer models of neutron scattering experiments - also including models of the sample materials - will be used on an everyday basis in the experiment planning, experiment control and data analysis.

2. Simulation packages. What has been done?

McStas and VITESS are two of the mostly used simulation packages in different neutron scattering laboratories worldwide.

The software package McStas (Monte Carlo Simulations of Triple Axis Spectrometer) is a complex software tool for neutron ray-tracing simulations for all kinds of neutron scattering instruments and facilities [2].

The package based on a meta-language has been specially designed for neutron simulations. Input parameters are written in this language and will be automatically translated into ANSI-C code. The present McStas version is 1.8, an update to the initial release in October 1998. The version 1.8 covers around 90 predefined components, which can be extended or updated by users. The McStas package can be downloaded freely from the McStas webpage [2]. The package is being developed by a core developer team of Risø National Laboratory and the Institut Laue Langevin. In addition, the developer team gets support by component developers, who are writing extensions or new components.

McStas can be operated under the common operating systems like Linux, Tru64 or Windows. The graphical user interface is written in Perl/PerlTK. The output files (simulation results) can be displayed using the widespread graphical tools Matlab, Scilab or Pgplot. The users can choose one of the named graphical tools.

McStas is highly accepted by the neutron scattering community which can be recognized from the long list of publications and simulated instruments [3].

The VITESS Monte Carlo package covers the same functionality as McStas. It has been developed and is continuously improved and extended at the HMI Berlin in the framework of the Spallation Sources project [4, 5].

VITESS truly has a modular structure in a sense that each module (each instrument part) works as an executable individual program reading in from the previous module and writing out the neutron trajectories which again will be read in by the next module. Development tends towards very complex systems. By using the “External command” function, the users can insert their own modules written by themselves. Operating systems are Windows, Unix SunOS, OSF1 or Linux. The graphical user interface is based on Tcl which works on all platforms.

VITESS has already been used for MC simulations of a wide range of instruments: beam extraction/guide systems, polarizing beam splitter, TOF backscattering, SANS; reflectometry, chopper spectrometers, powder diffraction, single crystal diffraction, triple-axis-spectrometry, NSE (pulsed), etc. VITESS has been earlier implemented in the framework of the ESS project. Nowadays it is used by a wide community.

3. Examples of complex systems

Recent developments of the McStas and VITESS Monte Carlo software packages for simulation of neutron scattering instruments allow for the computation of neutronic systems of very complex geometries.

For example, the module 'supermirror ensemble' in VITESS simulates a number of supermirror plane sections in any geometry, including spin dependent reflectivity and absorption. This module was intensively used in the optimization of the bi-spectral extraction system for the new guide hall of BENSC at HMI. It was also used for simulations of beam splitter polarizing cavities at BENSC. Another example is the module 'Fermi chopper' which simulates real 3-dimensonal slit packages with no analytic approximations which will be presented here [6-8]. We will also present here Monte Carlo simulation results of a time-focused pulsed source crystal analyzer spectrometer prototype [9,10]. In this short survey of VITESS results we focus on the results describing correlations of neutron coordinates, that is, two-dimensional diagrams as acceptance-, phase diagrams.

Another field of application is the use of the Monte Carlo packages for analyzing data during and after an experiment. In this case we are speaking about a ‚Virtual Experiment'. What we understand under a virtual experiment is a full simulation of a real measurement. The simulation should include all components beginning with the neutron source and finishing at the detector position. For the presented simulations the Monte Carlo program McStas was used. The goal is to show that a complex powder diffraction experiment can be simulated regarding both intensity and resolution [11].

Optimizing the design and improving the performance of a new neutron scattering instrument or upgrading of an existing instrument are presently the main fields of application of the Monte Carlo simulations.

For example, focusing techniques play an increasingly important role in neutron scattering due to the rather limited flux of the neutron sources and the advent of modern materials that can often only be produced in small quantities. Usually, doubly focusing monochromators in combination with doubly focusing guide tubes with linear tapering are used. The disadvantages of linear tapering are a very inhomogeneous phase space at the sample position and that the flux is decreasing with increasing distance from the exit of the guide tube. The example presented here shows a numerical optimisation using McStas of an advanced parabolic focusing supermirror device representing a major improvement [12, 13].

3.1 VITESS Fermi choppers

The module 'Fermi chopper' in VITESS simulates real 3-dimensonal slit packages with no analytic approximations. This module works with two options: straight and curved.

The 'straight' option is a Fermi chopper with straight channels i.e. the very fast neutrons are practically transmitted with only a time modulation and lower speed neutrons are modulated both in time of flight and wavelength. The 'curved' option is a Fermi chopper with curved channels i.e. neutrons are transmitted with a time and wavelength modulation.

A benchmark calculation for the curved Fermi chopper has been carried out for the slit packages of the HET spectrometer at the ISIS Facility [6,7]. The benchmark calculations show that the module is highly reliable and can be used for optimisation of Fermi chopper instruments. As it can be seen in the example in Figure 1, the experimental signal just behind the Fermi chopper can be well reproduced by the simulations and also by the analytical calculation [8].

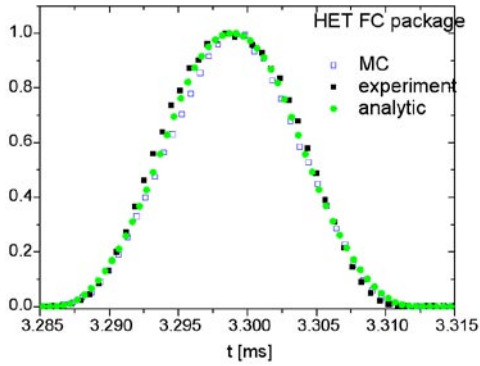


Fig. 1:
Time distribution behind the HET Fermi chopper, which was simulated exemplarily.

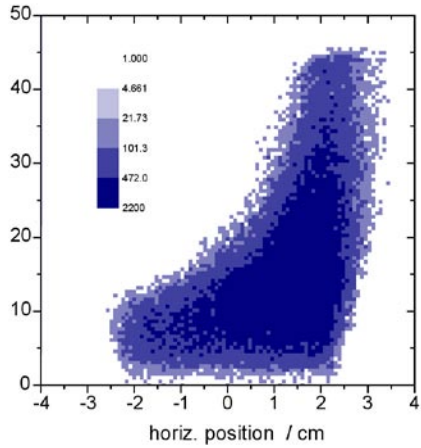


Fig. 2:
Horizontal position and wavelength acceptance diagram of the simulated straight Fermi chopper.

As a further example, we show the correlation between the horizontal position and transmitted wavelength (the rotation axis being vertical) for a straight Fermi chopper. The module describes a slit package consisting of straight silicon wafers with gadolinium layers on the wafer sides forming an array of transparent channels and absorbing walls. The width of the channel system is 6 cm, the length of the channels 1 cm, the number of channels is 100, the Gd-wall thickness 0.01 cm. The rotation frequency is 600 Hz. The cut-off wavelength given by the analytical approach corresponds to the limit at about zero horizontal position as it can be observed in the position-lambda diagram in Figure 2. However, neutrons are transmitted on the positive side with 40 Å and on the negative-position side the limit is less than the nominal.

The origin of this effect, for this type of wide but short-channel Fermi chopper, is the relative motion of the channels and neutrons to each other, once in the same and once in opposite direction [8].

3.2 Time-Focused Crystal Analyzer Spectrometer

Another example of MC simulations of complex geometry setups is about VITESS calculations of a pulsed-source time-focused crystal analyzer spectrometer which is planned to be realized in a test at IPNS.

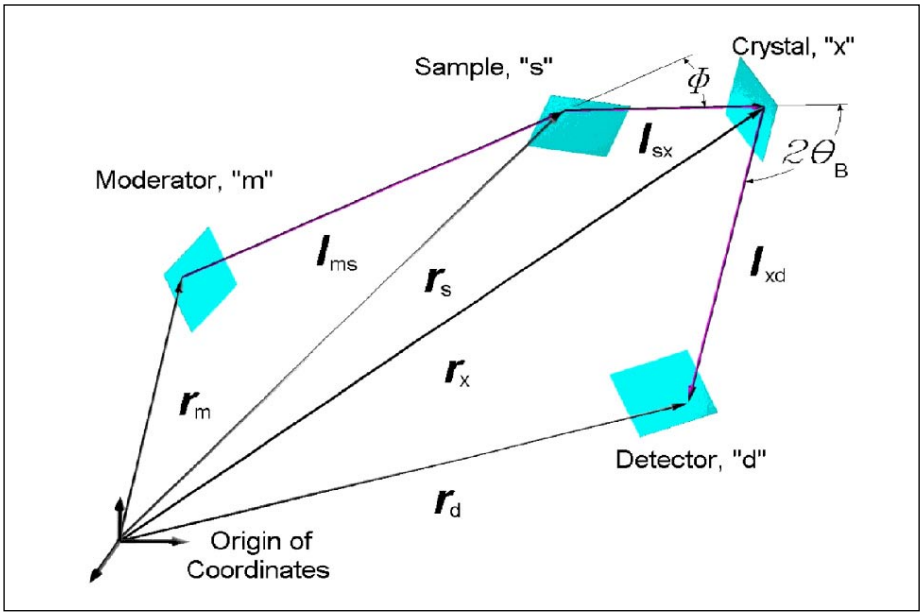


Fig. 3: Schematic layout of a pulsed-source time-focused crystal analyzer spectrometer.

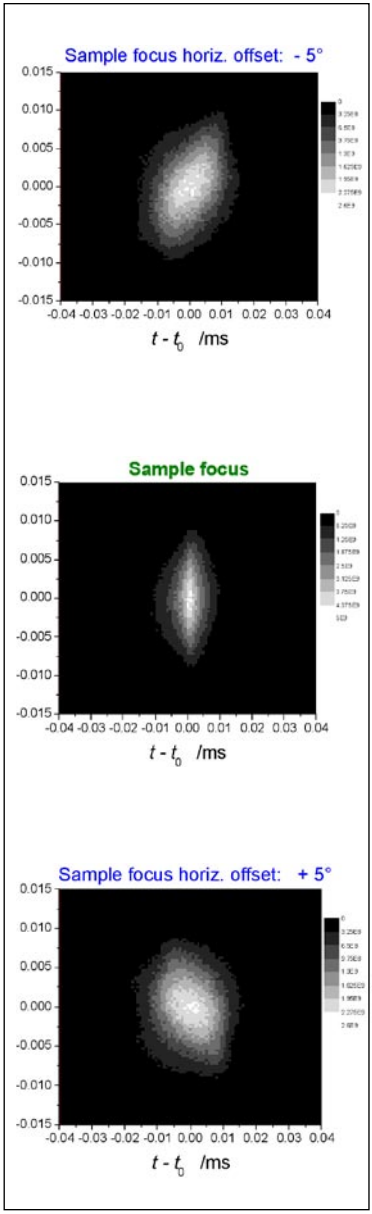


Fig. 4: Time-of-flight – wavelength diagrams showing the sample focusing effect at 60° elastic scattering angle.

The simulations are based on the linear vector theory of Carpenter et al. [9]. We checked the theory by simulations and also calculated in this way the non-linear contributions. The schematic layout of the geometry is shown in Figure 3. Moderator, sample, analyzer crystal and detector have the general positions $\mathbf{r_m}$, $\mathbf{r_s}$, $\mathbf{r_x}$, $\mathbf{r_d}$ in the coordinate system shown in the figure. These are represented by flat 2D rectangular elements, which can be rotated in space by allowing that the Bragg condition can always be fulfilled (by using off-cut crystals where the crystal surface and the diffraction planes do not coincide). The flight paths of different individual neutron trajectories between the spectrometer elements are labelled by the vectors $\mathbf{l_{ms}}$, $\mathbf{l_{sx}}$, $\mathbf{l_{xd}}$ [9].

In the results shown in the following figures, we set moderator, sample, crystal and detector two-dimensional and checked the correlation between the orientation of these elements and the shape of the signal in the detector as given by the linear theory. For each element one obtains a focusing condition from the theory. For example, in the case of the sample the following term has to be zero:

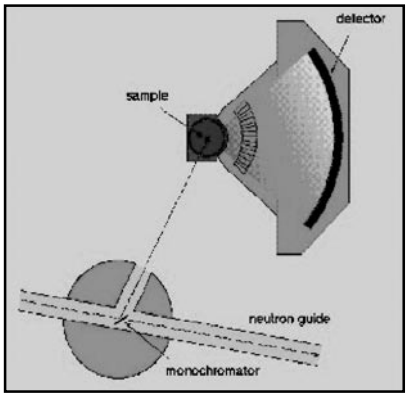
$$(\delta_s\ term) = \frac{1}{v_o}\left\{[(\lambda'_o/\lambda_o)\hat{\boldsymbol{L}}_1 - \hat{\boldsymbol{L}}_2] - \frac{1}{4L_2\sin^2\theta_{Bo}}[(\lambda'_o/\lambda_o)^3 L_1 + L_2 + L_3]\times \right.$$
$$\left. \times[(\cos 2\theta_{Bo})\hat{\boldsymbol{L}}_2 - \hat{\boldsymbol{L}}_3]\right\}\cdot\delta_s,$$

This means that the vector in the bracket has to be perpendicular to the relative coordinate vectors of the scattering points. The formulas of the focusing conditions can be obtained as described in [9].

The effect of focusing can be better understood by the time-of-flight wavelength diagrams [1] as shown in the Figure 4. The first diagram shows a horizontal offset from focus −5°, the second the focused orientation and the next a horizontal offset from focus +5°. The effect of focusing can be recognised in the tilting angle of the symmetry axes of the distributions.

3.3 Virtual experiment for the cold powder diffractometer DMC

As an example for a virtual experiment, the cold neutron powder diffractometer DMC at PSI has been chosen using the complex powder sample $Na_2Ca_3Al_2F_{14}$. The DMC is a flexible instrument with 400 sensitive BF_3 detectors (angular separation 0.2°) allowing for simultaneous measurements within a scattering angle range of 80°. The wavelength range is 2.3 Å to 6.5 Å. Figure 5 shows the basic design of DMC and the model designed with McStas.



Using this model, a real measurement on DMC with a sample $Na_2Ca_3Al_2F_{14}$ of size 10x30 (D x H) mm^2 has been compared with the Monte Carlo simulation. The results are shown in Figures 7 and 8. The comparison has been done for a number of 16 Bragg reflection peaks, including symmetrically equivalent reflections. The used wavelength was 2.567 Å. The simulated values are normalized to the maximum count rate of the measurement i.e. to the Bragg peak 71.92 ° shown in Figure 8.

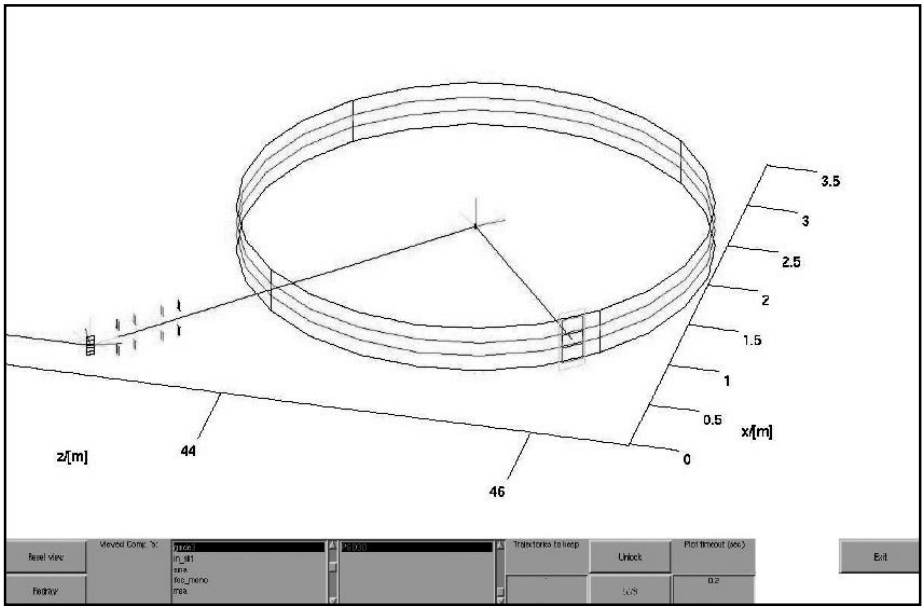


Fig. 5: Basic design of DMC (top) and the McStas model.

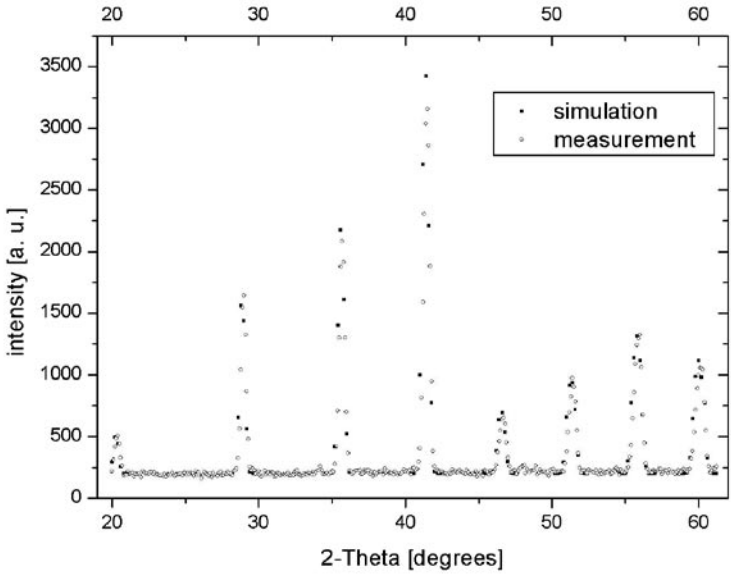


Fig. 6: Comparison of simulated and measured data: part 20° – 62°

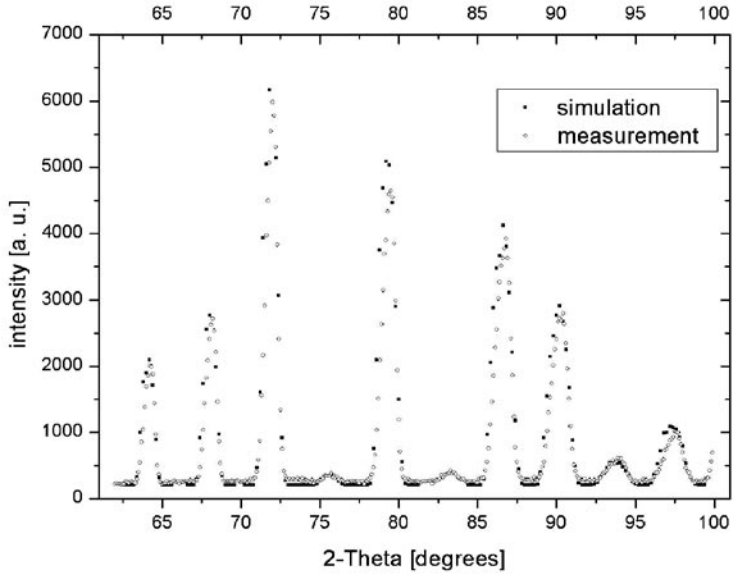


Fig. 7: Comparison of simulated and measured data: part 62° – 100°

The comparison shows that in addition to the exact peak position also the peak height and peak resolution agree very well. It is to mention that for some peaks in the Figures 6 and 7 several Bragg peaks do overlap, e.g. peak 79.36° contains four Bragg reflections. This overlapping could also be reproduced by the Monte Carlo simulations.

The comparison of computed and measured single peak resolutions (see Figure 8) demonstrates that simulated data can be used to evaluate with high precision the measured data. In case of Bragg peaks 28.98° and 51.4° the deviation in FWHM is approx 0.1°.

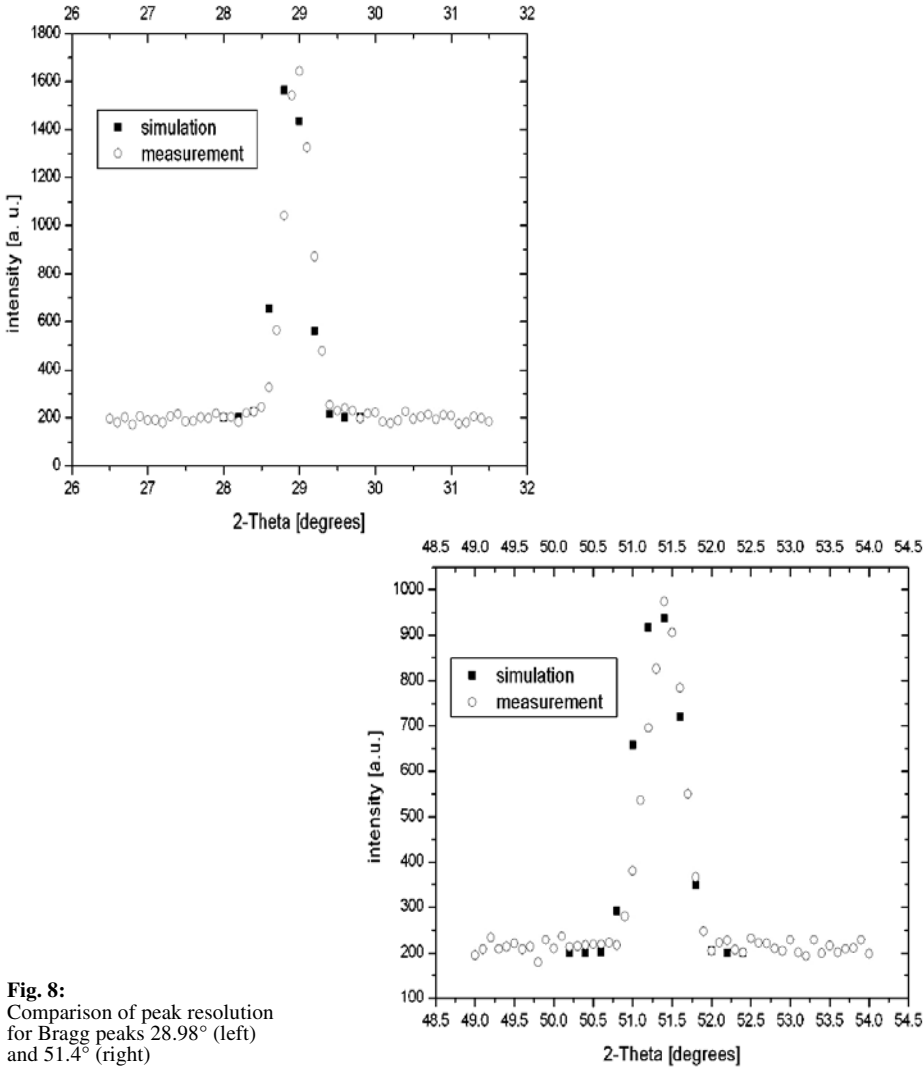


Fig. 8:
Comparison of peak resolution for Bragg peaks 28.98° (left) and 51.4° (right)

3.4 Design of an advanced focusing device

A design study for an advanced focusing device (AFD) has been done for the polarized triple-axes spectrometer TASP at PSI [11]. The AFD was situated between monochromator and sample position. The investigations were done for the cases of horizontal, vertical and horizontal/vertical focusing of the neutron beam. The goal was to demonstrate the possibility to shift the area of maximum intensity significantly far away from the exit of the guide. The investigations were carried out for different sample sizes, for different distances between monochromator and sample position, for different AFD lengths and different neutron energies. Of course, using a horizontal focusing supermirror device, the divergence of the neutron beam is increased. The consequence is that the q-resolution will be coarser. The calculated parameter sets covers the real conditions for TASP at the spallation source SINQ at PSI. The TASP instrument is positioned at the end of the cold neutron guide RNR14. The distance between the TASP monochromator and the cold neutron source is approx 54 m. The dimension of the neutron guide is 3.5 cm (width) x 12 cm (height). The used monochromator (PG002) can be only focused vertically in a neutron energy range of 2.1 to 25 meV. Figure 9 shows the comparison of calculated and measured wavelength spectrum at the TASP monochromator position.

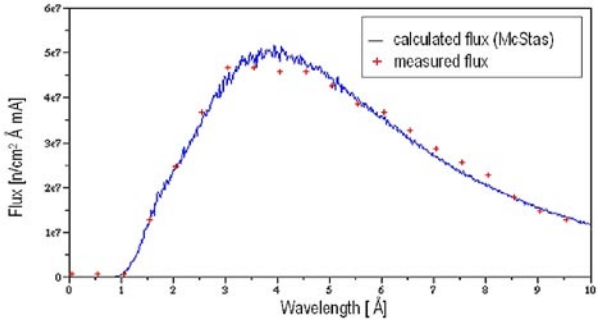


Fig. 9:
Available wavelength spectrum at the TASP monochromator position; comparison of calculated and measured spectrum

Generally, the McStas simulations have shown that the flux at sample position can be increased significantly using a parabolic tapering focusing guide. Figures 10a and 10b show the beam spot at sample position (1.8 m away from the monochromator position). In the case of focusing (10a) the flux maximum is higher and the homogeneous central area is smaller compared to the case without focusing (10b). The dimensions of the calculated trumpet are: length 1.3 m; entry height 0.12 m; entry width 0.035 m; focal point 0.3 m far away from the guide exit.

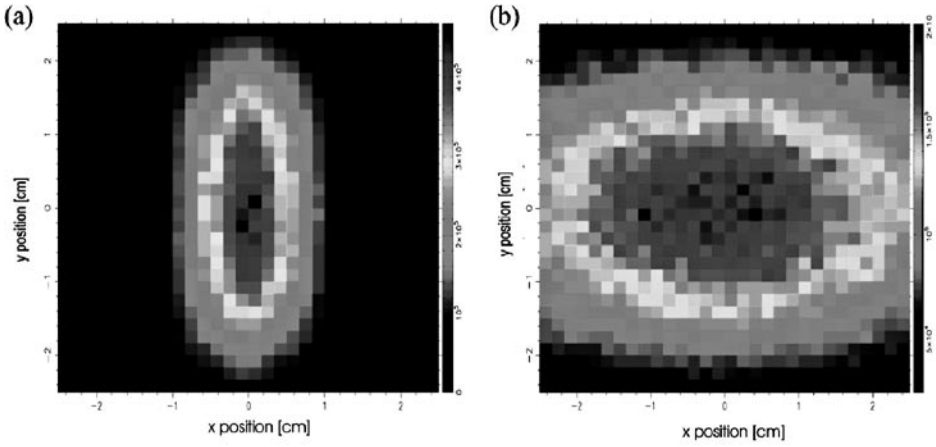


Fig. 10: Comparison of the beam spot at the sample position;
(a) with vertical / horizontal parabolic trumpet; (b) without trumpet

In principle, the focusing could be also achieved by linear focusing but the special effect of parabolic focusing is displayed in Figure 11a. It can be seen that the flux maximum is located at the focal point, 0.3 m away from the end of the trumpet. In case of linear focusing the flux is decreasing with increasing distance from the trumpet end.

The gain factors depending on the neutron energy are another point of interest. With the chosen TASP configuration and a sample size of 1 cm^2 a gain between 2.0 and 2.5 has been obtained for k_i between 2.1 and 1.2 $Å^{-1}$ (Figure 11b).

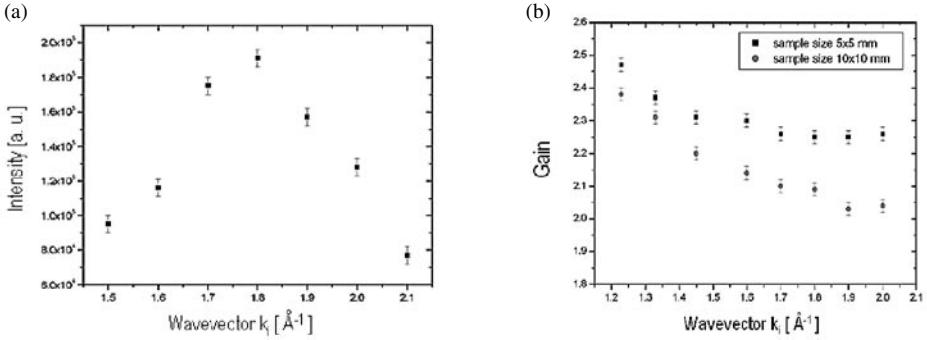


Fig. 11: (a) Flux after guide exit – focal point at 1.8 m after monochromator; (b) gain with focusing guide over a setup without trumpet for different neutron energies

4. Conclusions

The application of Monte Carlo simulations for designing and upgrading neutron scattering instruments has become a routine procedure by now. The simulation packages McStas and VITESS have been established as proven tools for this purpose. The use of the Monte Carlo simulations for data analysis (virtual experiments) has also made a big progress in the last years. It is foreseeable that data analysis using Monte Carlo technique will become a standard method.

Acknowledgement

McStas and VITESS are partially supported by SCANS (Software for Computer Aided Neutron Scattering) an RTD network within the Enhancing Access to Research Infrastructures activity of the Improving Human Potential program, part of the 5th and 6th framework program of the European Commission.

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Announcements

New SGN/SSDN Members

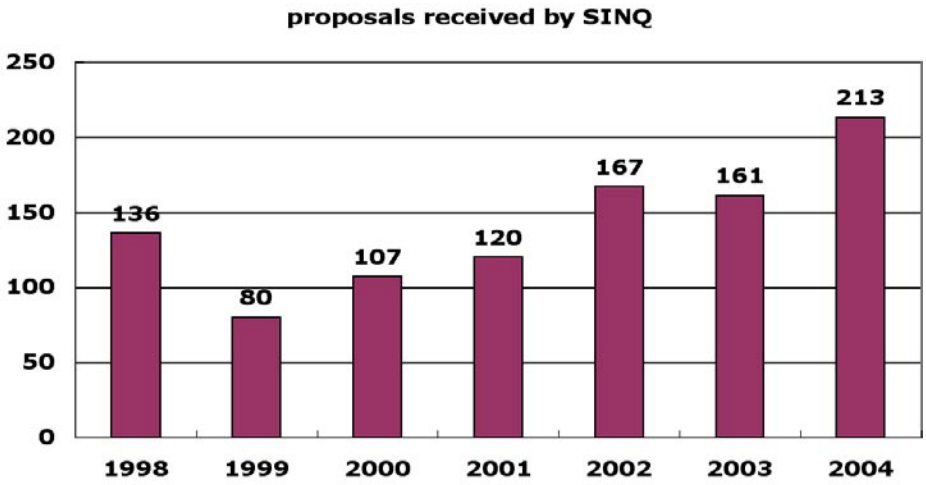
The Swiss Neutron Scattering Society welcomes six new members since the publication of the recent issue of 'Swiss Neutron News':

- R. Bercher (NUM department, PSI, CH)
- T. Geue (LNS, ETHZ & PSI, NUM department, CH)
- M. Könnecke (LNS, ETHZ & PSI, NUM department, CH)
- M. Knecht (User Office, NUM department, PSI, CH)
- M. Schneider (LNS, ETHZ & PSI, NUM department, CH)
- S. Shapiro (Brookhaven National Laboratory, USA)

Presently the SGN has 195 members.

News from SINQ

The recent SINQ deadline on 15/11/2004 again set up a new record of received proposals: the User Office counted 113 new proposals. Together with the May deadline totally 213 new proposals were submitted in 2004. 28 % came from Swiss groups, 48% from EU countries and associated states and 24% from 'the rest of the world'.



The figure above shows the development of the submitted proposals since 1998. Since the year 2000 the number has almost doubled. The strong impact of the available access funds (start of FP5 in 2002, FP6 in 2004) within the European framework programs is clearly visible.

In 2004 again almost 600 visits were made to SINQ (270 individual users) and more than 370 experiments were performed on the 10 instruments in user operation between May and December.

Open Positions at ILL

To check the open positions at ILL please have a look at the ILL-homepage: http://www.ill.fr following the link 'Job Offers'.

Symposium in honor of Albert Furrer

Joel Mesot
Laboratory of Neutron Scattering, Paul Scherrer Institute & ETH Zurich,
CH-5232 Villigen-PSI, Switzerland


H. U. Güdel

On October 6th, 2004, a symposium in honor of Albert Furrer was held at the Paul Scherrer Institute (PSI), Switzerland, to celebrate his retirement and 35 years of research at the fore front in neutron scattering. Over 150 participants from all over Europe attended the event, which was centered around entertaining presentations given by four prestigious collaborators of Albert Furrer. The symposium also nicely coincided with the 20th anniversary of the Laboratory for Neutron Scattering, a joint venture of ETH Zurich and PSI, which was created when Albert Furrer took the lead after the retirement of Walter Hälg from ETH Zurich. The first speaker, Hans Ueli Güdel from the university of Bern reported on 30-years of fruitful collaboration on the investigation of magnetic dimer-, trimer- and higher multimer-systems, documented by numerous high level publications. These examples perfectly illustrated the pioneering work of A. Furrer and H. U. Güdel in a field (quantum magnetism), a topic that during the last few years has returned to fashion. H. U. Güdel also underlined the huge impact A. Furrer has had due to his ability to attract and motivate young scientists. Two of the authors of the present report have benefited from this.

To be completely honest H. U. Güdel pointed out that this life-long partnership had suffered from Albert Furrer's infidelity caused by a successful excursion into the fascinating world of high-temperature superconductors. This particular chapter of Albert Furrer's work was highlighted in a very lively and enchanting manner by Karl Alex Müller (Uni. Zurich and IBM Rüschlikon) himself, the discoverer of superconductivity in the cuprates and 1987 Nobel price laureate in physics. Beside his remarkable scientific productivity Albert Furrer played a


AF, K. A. Müller, M. Steiner

K.A. Müller

leading role for the development of neutron scattering in Europe. This particular aspect was presented in great details by Prof. Michael Steiner (HMI). Aside from being active in numerous International Advisory Committees and Scientific Councils, Albert Furrer has been, for example, chairing the Scientific Councils of both the Hahn-Meitner-Institute and the Neutron Spallation Source AUSTRON. He has also been chairman and co-founder of the European Neutron Scattering Association. The final speaker, Peter Böni from the Technical University in Munich, devoted his talk to the advance of the Spallation Neutron Source SINQ at PSI with particular emphasis on the development of supermirrors for optical components like neutron guides and polarisers. A banquet followed the presentations featuring several presents and a brilliant after dinner speech by Bob Cywinski (Uni. Leeds), whose last words perfectly summarized the sentiments of the audience: we, the Swiss and European neutrons scatterers, are proud of you, Albert!

Caption: Three chairmen of the ENSA congratulate a fourth one: Albert Furrer (from left to right: F. Barocchi, D. Richter, AF, B. Cywinski).

P. Böni

B. Cywinski

Albert Furrer's Retirement

Peter Allenspach
Laboratory of Neutron Scattering, Paul Scherrer Institute & ETH Zurich,
CH-5232 Villigen-PSI, Switzerland

Albert Furrer's retirement at the end of November marks the end of an era for Swiss and international neutron scatterers. In all the neutron centers the first pioneering generation of scientists who started their career as neutron scatterers have retired or are leaving soon, which is of course connected to the start of most of the first research reactors in the late fifties and early sixties. Neutron scattering as a technique had to be developed both technically and scientifically and these last 40+ years have seen a tremendous dynamics in this field. We, as the following generation of scientists, can make full use of all the facilities, instruments and techniques resulting from their work. Albert, however, is outstanding in the sense that besides developing new techniques, doing excellent science, building a neutron source was also one of the few who took the lead to amalgamate the individual neutron scatterers into a community with common goals.

Albert made his appearance in the scientific community with a paper in 1965 with following title (in German): „Experimental proof of s-d interaction in fcc cobalt by means of spin wave scattering of polarized neutrons". Replacing cobalt by let's say an oxide-compound would make this title sound quite topical today by using the full potential of neutrons. Later he took the lead in measuring crystal field splittings of rare earths in different materials and in quantitatively analyzing the corresponding results (which is the major job and often causes problems still today). Crystal field effects again were important pieces in the puzzle of high temperature superconudctivity many years later. Another field of research he pioneered together with Hans Ueli Güdel was the investigation of magnetic clusters which again became topical many years later under the name molecular magnets. Hence, it is safe to say that Albert was always ahead of time and that he had a feeling for the important fundamental effects in condensed matter science.

P. Fischer

In the seventies Albert spent his postdoc years at Risø and Oak Ridge and than came back to Switzerland to do experiments at the reactor Diorit. Unfortunately, this reactor was shut-down shortly thereafter and he and his colleagues had to move to the reactor Saphir. In 1984. after the retirement of Prof. Walter Wälg, the Laboratory for Neutron Scattering (LNS) with Albert as its first head was founded. During this 20 years under his leadership the lab grew from 13 to 55 people, the new neutron source SINQ has been built and successfully taken into operation and a huge amount of excellent science has been done under his guidance.

The old and the new head of LNS: Albert together with his successor Joël Mesot.

W. A. Müller or C. Blocher?

Surely, all this was sufficient reason for celebrating him and his achievements. In October a symposium was held to cover the official part (see article by Joël Mesot in this issue). All the members of the laboratory had an additional opportunity to participate in a party for Albert in November, where many serious and less serious speeches were given, culminating in our present for Albert: a presentation by his favorite comedian Walter Andreas Müller impersonating Federal Councilor Christoph Blocher.

W. Hälg and AF

3rd Summer School on Condensed Matter Research, Zuoz, 7 – 14 August 2004

W. Fischer
NUM department, Paul Scherrer Institute

The special topic for this school was "Phase Transitions". While the theoretical part of this subject was presented on a rather general base, the experimental presentations emphasized the methods of neutron- and light-scattering as well as muon spin resonance.

About ninety participants attended the school, seventy of those were students on the post-graduate or post-doc level. The majority of the students had their origin mainly in western- and eastern European countries.

The school covered the theoretical and experimental aspects of phase transition phenomena. Special care was given to a thorough introduction to the basic principles (R. Morf, PSI and I. Tranquada, Brookhaven) including universality and renormalization groups (H.W. Diel, Essen) in order to prepare the students for the following lectures, which were somewhat more specialized. These covered the subjects:

- Critical and Multicritical Behaviour
  (J. Als-Nielsen, Copenhagen, H.W. Diel, Essen and R. Coweley, Oxford)
- Dynamics of Critical Phenomena
  (B. Halperin, Harvard and J. Als-Nielsen, Copenhagen)
- Structural Phase Transitions
  (S. Shapiro, Brookhaven)
- Glass Transitions
  (M. Müller, Rutgers and A. Keren, Haifa)
- Superfluidity and Superconductivity
  (M. Sigrist and H.R. Ott, ETH Zürich and J. Mesot, PSI)
- Quantum Phase Transitions
  (M. Vojta and Chr. Pfleiderer, Karlsruhe and Chr. Rüegg, PSI)

A special evening lecture by N. Straumann, University of Zurich, on Phase Transitions in the Universe, as an attempt to extend the horizon of the participants into cosmological dimension eased up the tough subject.

In view of the availability of a rather rich literature on this year's topic we decided to abstain from a production of proceedings on this school. However, thanks to the commitment of the lecturers we were able to provide the students "hand-outs" of the lectures at the beginning of the school.

This summer school was the last one that I had the pleasure to set up and organize together with Albert Furrer, both being due to retirement towards the end of the year. I hope we could establish some sort of tradition with the long series of schools earlier on "Neutron Scattering", now extended into the present set on "Condensed Matter Research". Personally I would be glad, having terminated my official professional activities to attend further schools in Zuoz as a student. Further successful events of this kind should be guaranteed not only by our successors, but also by the continuing participation of Renate Bercher as by now legendary secretary of the school.

The participants of the school gathered for a group photo in front of the 'Lyceum Alpinum' in Zuoz.

NOBUGS 2004 Conference held at PSI

Mark Könnecke
Laboratory of Neutron Scattering, Paul Scherrer Institute & ETH Zurich,
CH-5232 Villigen-PSI, Switzerland

From October 18-20, 2004 83 IT specialists from all major neutron, synchrotron and μSR facilities convened at PSI in order to attend the fifth installment of the NOBUGS series of conferences. NOBUGS is an acronym for New Opportunities for Better User Group Software. The aim of NOBUGS is to foster the collaboration between IT specialists working at the various facilities in order to provide better software for the respective user communities.

Prof. R. Eichler, the director of PSI, welcomed the attendees on Monday morning. From then on the three days were filled with numerous presentations and discussions covering the fields of software methodology, data acquisition, data analysis, instrument simulation WWW-access, protein crystallography and facility management. In total 54 oral contributions and 10 posters were presented.

Collaboration itself and the problems with jointly developed software projects were discussed too. It was felt that it would be easier to agree upon standards for data formats or instrument access rather then on concrete implementations.

From the presentations given some trends can be distilled: graphical user interfaces become common place even in data acquisition. Many systems presented were designed as frameworks extendable either through plugins or in a scripting language in order to allow for the varying demands of the user communities. In terms of programming languages Java is in the rise whereas python appears to be the most popular scripting language. WWW access to facilities, data acquisition, data and data analysis is another hot topic. Some stage setting work has been done to integrate the results of instrument simulations into both the data acquisition and the data analysis process.

Summing it up the participants enjoyed an inspiring and lively meeting. A new collaboration was started to define a common access language/component model for instruments. For more information please consult the NOBUGS 2004 WWW-page at: http://lns00.psi.ch/nobugs2004

Conferences and Workshops 2005

(an updated list with online links can be found here: http://sinq.web.psi.ch/sinq/links.html)

January

SμS Users' Meeting
January 19-21, 2005, PSI Villigen, Switzerland

7th SINQ Users' Meeting
January 27, 2005, PSI Villigen, Switzerland

February

ISIS Neutron Training Course
February 6-11, 2005, ISIS facility, Rutherford, UK

Neutron Diffraction Characterization of Mechanical Behavior
February 13-17, 2005, San Francisco, USA

36th IFF Spring School: Magnetism goes Nano: Electron Correlations,
Spin Transport, Molecular Magnetism
February 14-25, 2005, Jülich, Germany

Annual Meeting of the German Societies for Crystallography and Crystal Growth
February 28 - March 04, 2005, Cologne, Germany

March

2nd Annual Winter Neutron School
March 3-11, 2005, Los Alamos, USA

Nanotechnology Course Series, Spring 2005 European Program
March 21-24, 2005, Davos, Switzerland

April

Spring School on Supramolecular Chemistry
April 11-15, 2005, Centre Loewenberg, Murten, Switzerland

Symposium on Neutrons at the Frontier of Earth Sciences and Environment at the General Assembly of the European Geosciences Union
April 24-29, 2005, Vienna, Autria

ICANCS XVII, Conference on the International Collaboration on Advanced Neutron Sources
April 25-29, 2005, Santa Fe, USA

May

NSTI Nanotech 2005
May 8-12, 2005, Anaheim, USA

ICCS 2005, International Conference on Computational Science
May 22-25, 2005, Atlanta, USA

ACA 2005 one day powder diffraction software Workshop
May 28, 2005, Orlando, USA

June

LB11, The 11th International Conference on Organized Molecular Films
June 26-30, 2005, Sapporo, Hokkaido, Japan

August

4th PSI Summer School on Condensed Matter Research
August 14-21, 2005, Zuoz, Switzerland

XX Congress of the International Union of Crystallography
August 23-31, 2005, Florence, Italy

September

Diffusion Fundamentals I
September 21-24, 2005, Leipzig, Germany

November

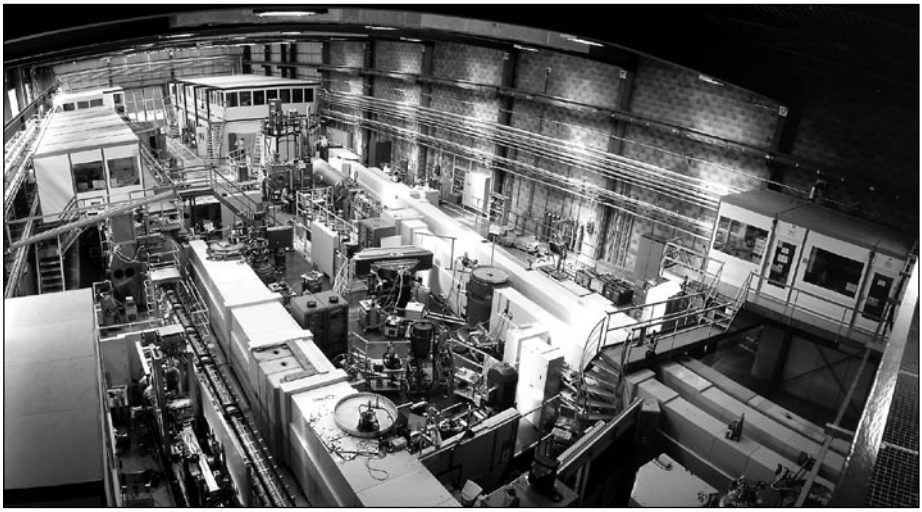
ICNS 2005
November 27 - December 2, 2005, Sydney, Australia

7th SINQ Users' Meeting

January 27, 2005
Paul Scherrer Institute

On January 27, 2005 the 7th SINQ users' meeting will be organized at PSI. The scope of the meeting is to inform the users about recent progress and developments around SINQ, to give them the opportunity to present their results and to exchange their ideas within the SINQ community. A poster session is not foreseen, instead it is planned to give as many users as possible the opportunity to report on their work in talks of typically 15 minutes in the parallel afternoon sessions. We especially encourage young scientists to participate and present the outcome of their research.

Further information on the program as well as registration forms can be found here: http://sinq.web.psi.ch/sinq/usmeet_7/meet7.html



SGN/SSDN General Assembly 2005

January 27, 2005, 17:00
Paul Scherrer Institute
OSGA/EG6 (Strahlenschutzschule)

Agenda:

1. Welcome
2. Minutes of the General Assembly 2004
3. Annual Report of the Chairman
4. Annual Report of the Treasurer
5. Report of the Auditors
6. Budget 2005
7. Change of Statutes (membership)
8. News from the European Neutron Scattering Association, ENSA
9. News from the Institut Laue Langevin, ILL
10. SGN/SSDN Activities 2005
11. Miscellaneous

All members are invited to attend the general assembly.
An online registration form is available here:

http://sinq.web.psi.ch/sinq/goto.php/duo/sinq/sinq_meet_register.php

Schweizerische Gesellschaft für Neutronenstreuung
Société Suisse pour la Diffusion des Neutrons
Swiss Neutron Scattering Society

Anmeldeformular / Registration Form

Name / Surname ……...

Vorname / First Name ……..

Akad. Titel / A cademic Degree ……....

Geschäftsadresse / Business Address ……...

……...

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Telefon / Phone …….

Fax ……

E-mail ……...

Privatadresse / Home Address ……..

……...

……...

Zustelladresse / Mailing Address: O Geschäft / Business
O Privat / Home

Datum / Date Unterschrift / Signature

…… ……...

Please submit to: **Paul Scherrer Institut, Secretariat SGN/SSDN,**
c/o Laboratory for Neutron Scattering, bldg. WHGA/147,
5232 Villigen PSI, Switzerland

PAUL SCHERRER INSTITUT PSI	**RESEARCH PROPOSAL** **Paul Scherrer Institut** *SINQ* Scientific Coordination Office 5232 Villigen PSI, Switzerland **phone:** +41 56 310 4666, **fax:** +41 56 310 3294 **email:** sinq@psi.ch, **web:** http://sinq.web.psi.ch	**SINQ** Swiss Spallation Neutron Source

Experiment Title:	**Proposal number** (to be completed by SINQ-SCO)

[ ] Short term proposal (next allocation period)	**[ ] Long term proposal (2 years)**

Proposer *(to whom correspondence will be addressed)* Name and first name: Address:	Phone: Fax: Email:

Co-proposer(s):
Name: Address: *(if different from above)* Phone/Fax/Email:

Sample description

Substance and formula: Mass: Size:

[ ] Polycrystalline [ ] Single crystal [ ] Multilayer [ ] Liquid [ ] Gas

Sample Container: Space group: Unit cell: a= b= c=

Area of Research

[ ] strongly correlated electron systems [ ] quantum spin systems [ ] superconductivity
[ ] structure [ ] dynamics [ ] magnetism [ ] materials science
[ ] polymer systems [ ] colloidal systems [ ] biological systems [ ] others

Hazard

Is there any danger associated with the sample or sample environment?
[ ] No [ ] Yes [ ] 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

[ ] New SINQ user [ ] New proposal [ ] Continuation of…….. [ ] Resubmission of……..

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: