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ON THE COVER:

The PSI "day of the neutrons" on October 28, 2007 attracted more than 3500 people. It was a great opportunity to present the neutron scattering and imaging activities at SINQ and turned into a big success for the whole institute, see article within this issue.

Contents

The President's Page

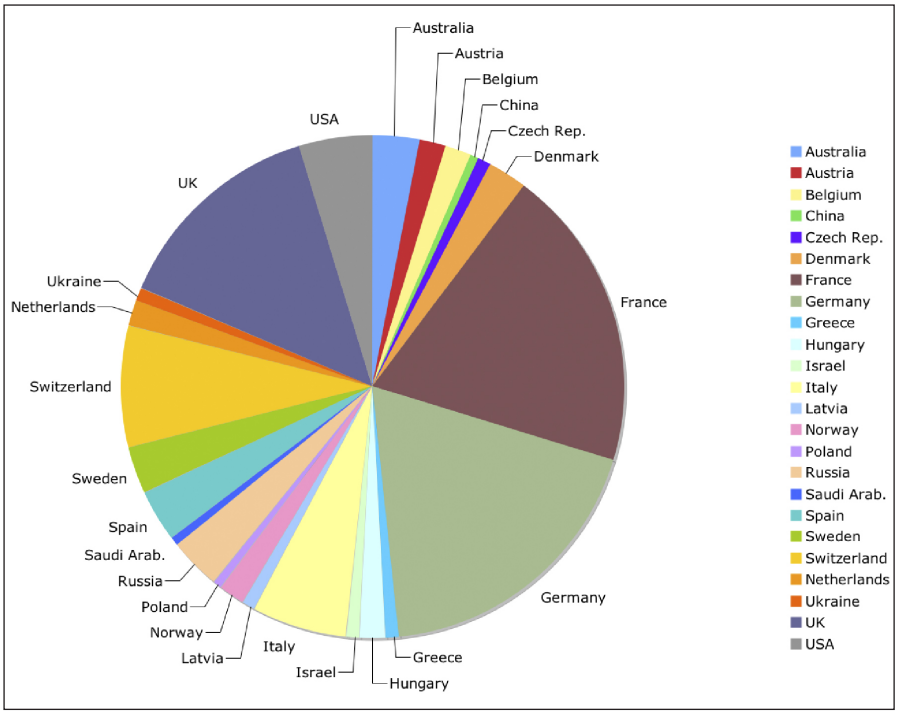
DEAR MEMBERS

ECNS'07 in Lund, Sweden, this summer was a very successful conference with a sizeable participation of Swiss neutron users and a very strong presence of speakers from Switzerland (see below). The last point is a very reliable measure for quality. I hope that the impact of the Swiss community remains in similar spheres for ICNS'09 in Knoxville, USA (May 3–9, 2009) and ECNS'11 in Prague, Czech Rep. (July 17–21, 2011). However, a high profile presence at topical conferences – outside of the "neutron club" – is of even higher importance for the individual scientist as well as the whole community in the view of a pending decision for ESS. An EU-FP7 ESS preparatory phase project which should help to pave the way towards a decision is expected to be signed still this year. I'm coordinating this project as ENSA chairman together with a team of three from the official site candidates (C. Carlile for LUND, F. Mezei for Hungary and J. Urrutia for Bilbao). The coordinating organization is PSI.

During summer and fall PSI kindly organized a symposium to celebrate 10 years of fruitful SINQ operation and a "Tag der Neutronen" to inform the population about neutron scattering and some of the corresponding research. Reports of these two very successful events can be found in this issue.

The 16T-magnet project, initiated by SGN and jointly funded by the Swiss government, PSI, MaNEP and SNS, is slightly ahead of schedule with a design review on January 24, 2008. Delivery to SNS will be in the first half of 2009 when SNS is expected to surpass ISIS by far in regular user operation. Hence, a ideal moment for Swiss users to have their first experience with this new source together with the new magnet.

Peter Allenspach



Country distribution of speakers at ECNS'07 in Lund.

Dynamics of Room Temperature Ionic Liquids by Means of Quasielastic Neutron Scattering

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INTRODUCTION

Room temperature ionic liquids (RTILs) are salts with melting points well below room temperature. They possess very interesting properties like extremely low vapor pressure, excellent thermal and electrochemical stability, very good dissolution properties for many organic and inorganic compounds, and low flammability; they are possible candidates as electrolytes for lithium batteries and fuel cells and for many more applications [1].

Apart from these applications and interesting chemical properties RTILs show a very rich physical behavior, like solid-solid phase transitions (order – disorder phase transitions), plastic crystalline phases with rotational degrees of freedom of the involved ions, and glass transition. Up to now only little is known about these phase transitions and about the dynamics within the liquid and plastic crystalline state. While many theoretical investigations are under way the experimental side is hardly explored. The preferred theoretical tool to examine the dynamical processes in RTILs is molecular dynamics simulations. On the experimental side there exist reports on experiments using PFG-NMR. To our knowledge only a few papers are dealing with neutron scattering experiments on ionic liquids [2-5] exist so far. The system under investigation within the mentioned papers was always an imidazolium based RTIL ([bmim][PF6], 1,3-dimethylimidazolium chloride).

In recent years a number of simulations have been done on ionic liquids. Most simulations again deal with imidazolium-based ionic liquids while papers concerning simulations on ionic liquids with other cations are very rare.

SAMPLE PREPARATION

Here we report on experiments on pyridinium-based ionic liquids. We now describe the synthesis of the liquids we used.

Preparation of n-butylpyridinium-chloride

To prepare n-butylpyridinium chloride, pyridine was refluxed in a standard reflux apparatus, fitted with a drying tube, containing P_2O_5. An

equi-molar quantity of 1-butyl Chloride was slowly added and the reaction mixture was refluxed in the dark for 4 days. After cooling to room temperature, the product was crystallized from EtOAc, filtered under vacuum, washed wit EtOAc and quickly transferred to a bottle, while still moist with solvent. The excess of solvent was then removed under vacuum at 50 °C for 24 h; yield: 87 %.

Preparation of deuterated and half-deuterated samples of n-butylpyridinium-chloride

Deuterated and half-deuterated samples, n-butyl (d9) pyridinium, n-butylpyridinium (d5) and n-butyl (d9) pyridinium (d5) were prepared analogously, using corresponding reactants.

Preparation of n-butylpyridinium bis (trifluoromethanesulfonyl) imide

Equi-molar quantities of n-Butylpyridinium-chloride and Lithium bis (trifluoromethanesulfonyl) imide were dissolved in DI water. The two solutions were added to a separatory funnel. The mixture was thoroughly shaken, the organic phase separated and washed with ID water for 5 times. The inorganic layer was extracted with CH_2Cl_2. Then the organic phase was concentrated under reduced pressure at 50 °C for 24 h and afterwards dried for 24 h under vacuum. Yield: 97 %

Preparation of deuterated and half-deuterated samples of n-butylpyridinium bis (trifluoromethanesulfonyl) imide

Deuterated and half-deuterated samples, n-butyl (d9) pyridinium bis (trifluoromethanesulfonyl) imide, n-butylpyridinium (d5) bis (trifluoromethane-sulfonyl) imide and n-butyl (d9) pyridinium (d5) – bis (trifluoromethanesulfonyl) imide were prepared analogously, using corresponding reactants.

Within this paper we report on experiments on 1-butylpyridinium Bis (trifluoromethanesulfonyl) imide (denoted as [bpy][Tf2N]). The schematic structure of the ions is shown in Figure 1 a), b):

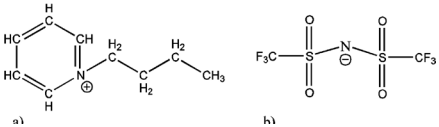

Figure 1: a) N-butylpyridinium cation and b) Bis (trifluoromethanesulfonyl) imide anion.

This ionic liquid belongs to a new class of RTIL with even better properties than those described in the introduction. The thermal stability is excellent and these liquids are really hydrophobic.

NEUTRON SCATTERING EXPERIMENTS

The experiments were performed on the time-of-flight spectrometer FOCUS [6] at SINQ. We used an incident wavelength of $\lambda i = 6$ Å, corresponding to an incident neutron energy of about 2.27 meV together with a PG 002 monochromator. At this wavelength the Gaussian resolution has a FWHM-value of 35 to 60 μeV. The sample was examined at different temperatures ranging from room temperature up to 460 K. For these measurements we used a closed cycle refrigerator. The sample was contained in a flat aluminum cell sealed with Pb-wire (the sample thickness was 0.2 mm in order to minimize multiple scattering). For calibration purpose a 1 mm thick vanadium slab was measured at 300 K for 4 h. Finally

the empty sample container was measured as background for the sample measurements.

DATA REDUCTION AND ANALYSIS

The collected TOF-QENS spectra were analyzed between -1 and 1 meV using the DAVE package [7]. This software allows for sample absorption and background corrections as well as for taking into account self-shielding effects and detector efficiency. The data have been binned into 12 Q-groups (Q_{min} = 0.45 Å^{-1}, Q_{max} = 1.55 Å^{-1}). The experimental data contain both elastically and quasi-elastically scattered neutrons. The former correspond to immobile (on the experimental time scale) species while the later result from species undergoing non-periodic dynamical processes. With this physical picture we used the following dynamic structure factor S(Q,E) [8, 9] to describe the data

$$(1)\quad S(Q,E) = e^{-\langle u^2\rangle Q^2/3}\{A_0(Q)\delta(E) + [1 - A_0(Q)]L(Q,E;\Gamma)\}$$

The first term $e^{-\langle u^2\rangle Q^2/3}$ is the usual Debye-Waller factor taking into account high-frequency periodic motions (oscillations). The delta-function accounts for elastically scattered neutrons either on atoms/molecules that are too slow for the experimental time window or immobile (fixed), while the Lorentzian L(Q,E;Γ) describes the motions of molecules (translational and/or rotational (re-orientational) types of molecular motions). The experimental measured spectra $S_{exp}(Q,E)$ are then given as

$$(2)\quad S_{exp}(Q,E) = S(Q,E) \otimes R(Q,E)$$

where R(Q,E) is the instrumental resolution function as measured with a vanadium slab (with the same geometry as the sample, thickness = 1 mm).

Figure 2 shows the linewidths at half maximum of the Lorentzian as function of Q^2; the corresponding experiment has been done at 380 K

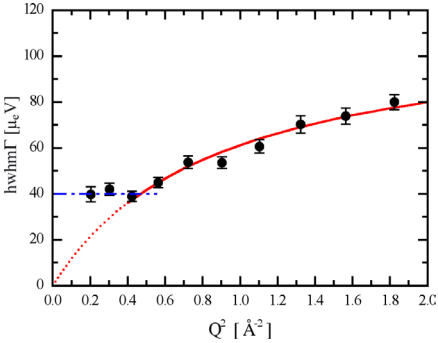

Figure 2: Plot of HWHM Γ vs. Q^2 at T = 380 K. Shown is the plateau at low Q^2 and the random jump behavior at higher Q^2 indicating a random jump diffusional behavior.

Up to Q^2 = 0.4 Å^{-2} we find a constant linewidth while at Q^2 > 0.4 Å^{-2} the linewidth increases according to a simple jump diffusional behavior. This finding is quite remarkable and indicates a dynamical process occurring within a confining region. Volino and Dianoux [10] made a model accounting for such a confined diffusional motion. According to their model the linewidth of the Lorentzian remains constant for Q < Q*≈3.3/R and for Q > Q* an increase of the linewidth can be observed. Here R denotes the radius of the confining region (assumed to be of spherical symmetry). The elastic incoherent structure factor (EISF) for this model reads

$$(3)\quad A_0(Q) = \beta + (1-\beta)\left[\frac{3j_1(QR)}{QR}\right]^2$$

where β accounts for the immobile fraction

of species and j_1 is the spherical Bessel function of order one. Immobile here means that these particles (ions) do not move on the experimental time scale. In Figure 3 we present the EISF as function of Q for three different temperatures.

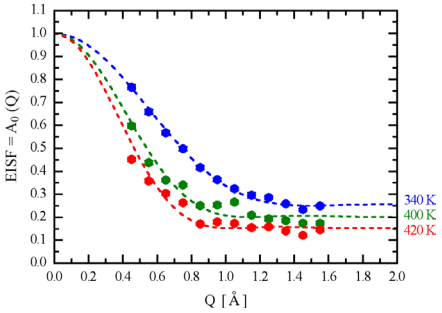

Figure 3: EISF vs Q for three different temperatures. The dashed curves are fits according to Eq. 3 with β and the radius of the confining region R as fit parameters.

From Figure 3 it's clear the measured EISF doesn't go to zero for high Q values; this experimental finding can be described by the factor β as already mentioned. β itself depends on the temperature as shown in Figure 4:

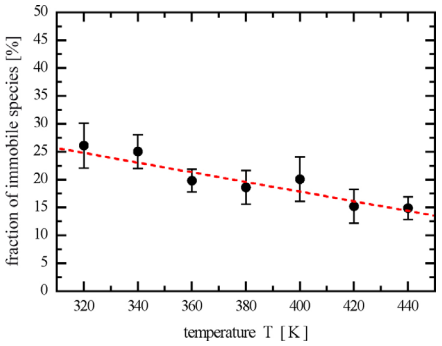

Figure 4: Fraction of immobile species as seen on the experimental time scale as function of temperature T. With increasing temperature this fraction decreases, thus more and more species contribute to the dynamic process.

With increasing temperature the fraction of immobile species β decreases, thus more and more species take part on the dynamical process. One can at this stage speculate about the nature of these immobile particles. A possible explanation could be the formation of ion-pairs (or even some large clusters). The diffusion coefficient of ion pairs will be smaller leading to a dynamics that is accordingly much slower and thus not detectable within the imposed experimental configuration.

The spatial extend of the confining region depends on the temperature as well, as shown in Figure 5:

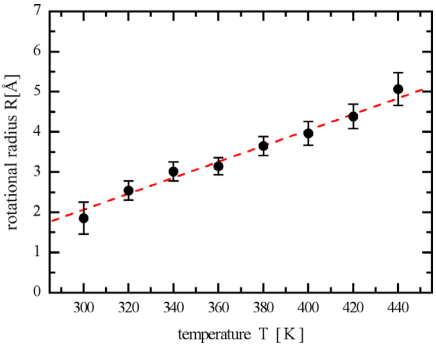

Figure 5: Rotational radius R, i.e., the radius of the confining region vs temperature deduced from fitting the EISF curves with Eq. 3.

with increasing temperature the confining region becomes larger. From the random jump diffusional behavior that is seen for Q > Q*, the short time diffusion constant can be deduced from the HWHM-values according to the model proposed by Hall and Ross [11]: $\Gamma(Q)=\hbar DQ^2/(1+DQ^2\tau_0)$ with the diffusion constant D and the residence time between successive jumps τ_0;the corresponding results are displayed in the following Figure 6:

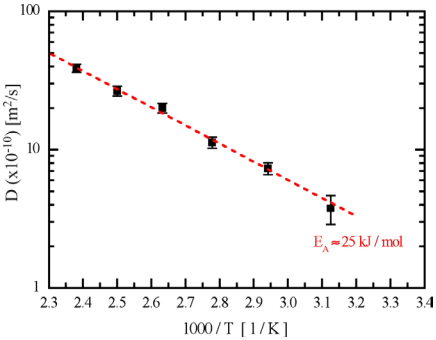

Figure 6: Diffusion coefficient (short-time diffusion coefficient for the dynamics inside the confining sphere) as function of inverse temperature. The data points result from fitting the region Q>Q* with the random jump diffusion model according to Hall & Ross. An Arrhenius-type relation for D(T) yields an activation energy of about 25 kJ/mol.

The diffusion coefficient as function of the inverse temperature shows a clear Arrhenius-type behavior with an activation energy of about 25 kJ/mol = 259 meV. This diffusion coefficient describes the diffusional motion inside the confining region.

RESULTS AND DISCUSSION

Up to now the main technique used to determine the self-diffusion coefficient of the cations and/or anions in ionic liquids has been pulsed field gradient nuclear magnetic resonance spectroscopy (PFG-NMR). However one has to keep in mind that this technique probes dynamic processes on microsecond time scale and has therefore a poor sensitivity to localized dynamics on the molecular scale (in space and time). QENS on the other hand isn't able to provide the same mesoscopic scale information as PFG-NMR but probes dynamic processes on the pico-second time scale and on molecular length scale. Therefore it is quite natural that both methods provide different diffusion coefficients [12] (long-time and short-time diffusion coefficients, respectively). With the help of the NMR-technique it is not possible to detect these confining regions due to just the different length-scale that is probed by this experimental method. Nevertheless a combination of these two experimental methods, i.e., NMR and QENS, on the same samples would give a deeper inside into the dynamics occurring in these ionic liquids.

In the liquid analyzed so far at a wavelength of 6 Å we see a very interesting dynamics of the cation. From our data analysis according to the Volino-Dianoux model of diffusion inside a confining sphere we could determine the spatial extent of this confining region and the fraction of immobile species. This fraction of immobile species decreases with increasing temperature indicating a thermally activated process. A possible explanation of these non-diffusing particles could be related to formation of ion-pairs (or even larger clusters) and with increasing temperature some of these previously formed pairs loose their connection and contribute therefore to the dynamic process we are probing with neutron scattering.

Our experimental finding concerning the motion of a cation inside a confining sphere is supported from results obtained with MD simulations performed by the group of Müller-Plathe [13]. This group found a cage-like effect in immidazolium-based ionic liquids: the cation is inside a cage formed by surrounding anions and the escape time the cation needs to jump outside this cage is in the range of hundreds of pico-seconds. The cage formed by the anions is due to strong electrostatic interactions between the cations and the anions.

OUTLOOK

We have just started with neutron scattering experiments on RTILs. With the preparative skill now available in our group at Saarland University we want to extend our research on RTILs with increasing length of the alkyl side-chain attached to the pyridinium ring. The question here is, how do structure and length of the alkyl chain influence the dynamics on the time- and space-scale that can be explored with quasielastic neutron scattering.

Another issue we want to analyze is the water dynamics within RTILs. This is due the fact that measurements of the dynamic viscosity as function of the fraction of added water revealed a very interesting findings, shown in Figure 7:

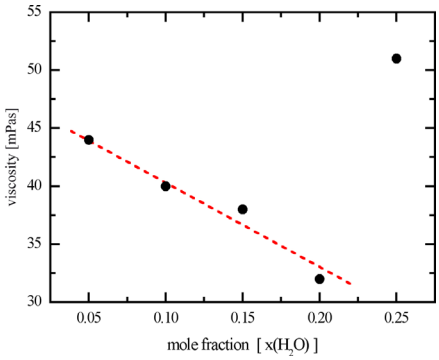

Figure 7: Dynamic viscosity as function of the mole fraction of water added to the neat ionic liquid n-pentylpyridinium Tf_2N.

In Figure 7 we show the dynamic viscosity as function of the added water content. At a mole fraction of 0.25 the previously decreasing viscosity seems to increase suddenly. A possible explanation could be the formation of water clusters or ion-water clusters within the sample leading to some kind of network above a percolation limit thus yielding a sudden increase of the viscosity. Quasielastic neutron scattering is a method that enables us to track the water dynamics on a molecular spatial and temporal scale within fully deuterated RTIL samples.

ACKNOWLEDGEMENT

We gratefully acknowledge financial support form the German Science Foundation DFG (DFG Priority Program SPP 1191 ***Ionic Liquids***) and the possibility to discuss with colleagues working in the field of ionic liquids at the 1st annual meeting of the above mentioned priority program held in Bamberg (12.–14. 12.2007). It's also a great pleasure to thank the people from DAVE team at NIST for their help and modification they made with respect to the analysis package DAVE.

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Discovering the Secrets of Antiferromagnetic Nanoparticles

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We present some of the highlights of our research on antiferromagnetic nanoparticles, performed at SINQ. Neutron diffraction shows the effect of particle size and inter-particle-interaction on the magnetic structure, while inelastic neutron scattering reveals the rich magnetic dynamics of these systems.

The agreement between PSI and Risø in 2001 resulted in the positioning of two instruments, RITA-2 and SANS-2 at the (then) newly inaugurated SINQ source. Furthermore, the agreement initiated a scientific collaboration, which is still evolving.

This article is the first of a series, which will present the outcome of the two instruments and the Danish-Swiss collaboration in general. The topic of the present article is the magnetism of nano-sized particles.

All work presented in this article was performed at RITA-2 and DMC. The research has so far resulted in 11 articles; see e.g. [1–6], while another 5 articles are underways.

PARTICLE SIZE, CRYSTALLINE, AND MAGNETIC STRUCTURE

In standard textbooks, the Bragg law is derived assuming the crystal to be infinite. For a nanoparticle, this does not hold. The result is a broadened diffraction pattern, where the peak widths are inversely propotional to the particle diameter.

Figure 1 shows neutron diffraction data on nanoparticles of the common iron oxide hematite (α-Fe_2O_3). Compared to diffraction data on a "normal" micrometer sized hematite powder, the line broadenings are pronounced. For this data, the line widths are transformed into an average particle size of 7 nm. This value is confirmed by transmission electron microscopy (TEM), which also shows the nice crystallinity of the particles; see insert to Figure 1.

The two inner diffraction peaks at q=1.37 $Å^{-1}$ and 1.50 $Å^{-1}$ (marked by *) stem from the antiferromagnetic order of hematite, while the other peaks (marked by *) are the structural peaks.

The intensity of the magnetic peaks reveal an important difference between nano- and microparticles. In the latter, the peak at q=1.37 Å^{-1}, almost disappears below 263 K, as seen in Figure 1. This proves that the moments turn to point along the c-axis (the Morin transition). For nanoparticles of sizes below 20 nm diameter, the Morin transition is absent.

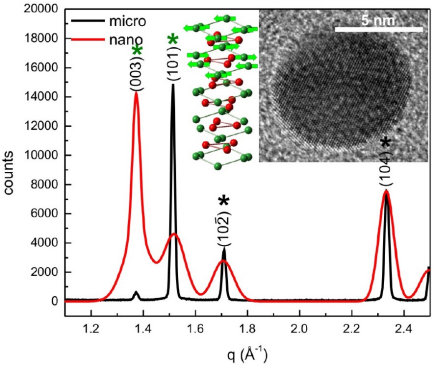

Figure 1: Neutron diffraction data taken at 20 K for micrometer sized and 7 nm diameter hematite particles. The TEM picture (top right) shows a perfect crystalline hematite nanoparticle on a carbon film. The crystal model (top) shows the arrangement of the oxygen atoms (red) and iron atoms (green). The arrows show the simple antiferromagnetic structure of the nanoparticles with alternating ferromagnetic layers along the vertical direction (the c-axis). The two lowest peaks are the antiferromagnetic ones. See discussion in the text.

INTER-PARTICLE INTERACTION

Nanoparticles have a surprisingly large surface. For example, 1 cm^3 diameter spherical particles of 10 nm diameter have a surface of 400 m^2. Hence, there is a large potential for surface interaction in a powder of nanoparticles, e.g. by direct contact between the electronic orbitals of the surface atoms of neighbouring particles.

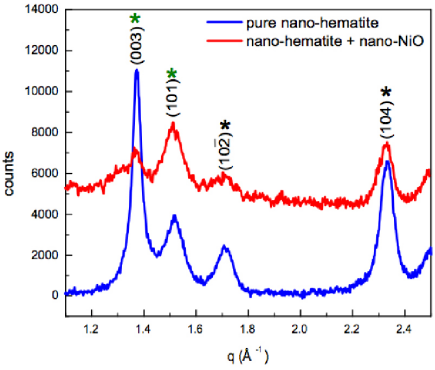

Figure 2: Diffraction data at 20 K of pure hematite nanoparticles and a mixed sample of hematite and NiO nanoparticles. Addition of the NiO particles are seen to causes a suppression of the magnetic hematite peak at q=1.37 Å^{-1}. From [1].

Figure 2 shows low temperature diffraction data from a sample of pure hematite nanoparticles (red) and a mixture of hematite and antiferromagnetic NiO nanoparticles (blue). In contrast to the pure sample, the hematite particles in the mixed sample clearly show a Morin transition [1]. This effect is still not understood in detail, but we presume that is caused by magnetic exchange interaction between the surface atoms in the two types of nanoparticles.

Another interaction effect is seen in pure samples of small (7 nm) hematite nanoparticles. Figure 3 shows that the innermost magnetic Bragg peak is significantly sharper than the other (magnetic or structural) peaks. This indicates that the magnetic correlation length along the c-axis is around 3 times longer than the size of the particles themselves [2]. TEM pictures taken later on frozen suspensions of nanoparticles show indeed this, as seen in Figure 3. A closer analysis of the crystal orientation reveal that the particles stack along

the c-axis. The magnetic interaction between surface atoms then in turn cause alignment of the magnetic order along this axis [2].

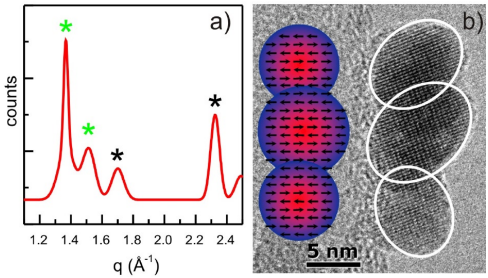

Figure 3: Magnetic correlation in hematite nanoparticles: a) neutron diffraction data shows a narrow (003) Bragg peak. b) TEM picture of chained particles, including a model of the magnetic structure along such a nano-chain. From [2].

MAGNETIC DYNAMICS OF NANOPARTICLES

In nanoparticles, spin waves of very long wavelength (low q) do not exist due to the finite size. Hence, the lowest q>0 spin waves can have energies of several meV. At low temperatures, the thermodynamics is thus dominated by the q=0 excitation mode, which has a non-zero energy due to the uniaxial size/shape anisotropy [7]. This mode can be visualized as a collective precession of all spins in the effective anisotropy field, see Figure 4. This mode is in nanoparticles often denoted "collective magnetic excitations" (CME).

In hematite, the magnetic interaction is particularly strong, reflected in the unusually high Neél temperature of 950 K. As a consequence, the spin wave dispersion is very steep, and excitations with q>0 have never been observed. The CME modes vere directly observed by inelastic neutron scattering on RITA-1 at Risø [8], and the RITA-2 spectrometer is particularly good for these studies [4–6]. Figure 4 shows a typical data set; the CME signal is seen as the two shoulders at 0.5 meV, on the side of the strong elastic peak, which in fact is the magnetic Bragg peak.

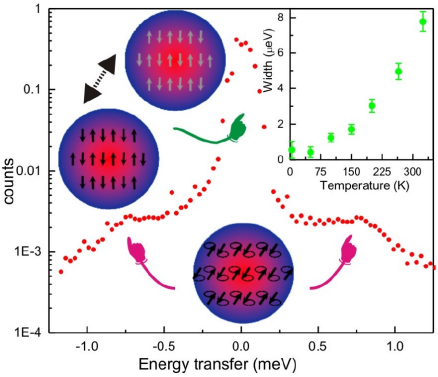

Figure 4: Inelastic neutron data on 8 nm hematite particles at 190 K, taken at q=1.37 Å-1 . Pink pointers mark the signal from CME, while the green pointer mark the elastic Bragg peak. The insert shows the temperature dependence of the broadening of the Bragg peak due to superparamagnetism. Data taken from [3].

Thermal excitations will cause more than spin precession. At random, the spins may, collectively, climb the energy barrier caused by the anisotropy, to reverse their direction. This is illustrated in Figure 4. This effect is denoted *superparamagnetic relaxation,* and is seen in neutron scattering as a quasielastic broadening of the elastic Bragg peak due to the finite lifetime. The temperature variation of this broadening is shown in Figure 4. It corresponds well to an Arrhenius behaviour, expected for thermal activation over an energy barrier [3].

WHY STUDY MAGNETIC NANOPARTICLES?
The world of nanoscience is fundamentally interesting, since it is allows the investigation of the transition between the atomic-scale world ruled by quantum mechanics, and the macroscopic world ruled by classical mechanics. At the nano-scale, one may encounter completely new phenomena, as in this example collective magnetic excitations and superparamagnetism.

Furthermore, magnetic nanoparticles have a number of applications, e.g. data storage (tapes or disk drives), where the direction of magnetization of ferromagnetic nanoparticles determines the value of the individual bits. In this case, superparamagnetism must be avoided, since it would cause decay of the stored data. Magnetic nanoparticles have other applications like part of novel composite magnetic materials, in spintronics, and for controlling drug delivery.

Finally, magnetic nanoparticles occur in nature, e.g. as components of soils, as compass organs in certain birds and bacteria – and they may be responsible for unresolved magnetic properties of minerals and on the planet Mars.

In conclusion, there are numerous reasons to investigate the magnetic properties of nanoparticles, and neutron scattering is one of the very good tools to obtain the information needed.

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The four Danish authors have been supported by a research grant from the Danish Research Foundation for Technical Sciences, shared between Technical University of Denmark, University of Copenhagen, and Risø (then an independent laboratory).

From left: Cathrine Frandsen, Luise Theil Kuhn, Kim Lefmann, and Christian R.H. Bahl.

The Time-of-Flight Diffractometer POLDI at SINQ for Material Sciences and Residual Stress Analysis

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The time-of-flight diffractometer POLDI at the continuous spallation source SINQ is in operation since 5 years. The instrument concept uses a novel multiple frame-overlap technique, which allows tuning to high intensity and high resolution simultaneously. It is designed to determine locally lattice spacings with high accuracy. The main applications are residual stress determination within engineering specimen and investigations of multi-phase materials.

INTRODUCTION

The requirements for most experiments in material science as well as for the determination of residual stress in engineering specimen are quite similar: high resolution in lattice spacings, good spatial resolution within a sample and the option to measure at a fixed scattering angle. The latter is of importance, since, in general, the lattice spacing will be dependent on the orientation. These requirements are not very well fulfilled with typical diffractometers for structure analysis at continuous neutron sources. Therefore, a special instrument for material and engineering sciences has been installed at SINQ.

At continuous neutron sources conventional time-of-flight (tof) diffractometers have a disadvantage in intensity compared to constant wavelength diffractometers. At conventional tof-diffractometers choppers prevent that neutrons of a certain pulse can catch up with neutrons of previous pulses. In a pulse overlap diffractometer this restriction is dropped. It is more than 20 years ago that Cockcroft and Kearley proposed a pulse overlap diffractometer for structure analysis [1] in order to increase the intensity.

At POLDI we developed a method which is adapted to the special requirements of a strain scanner [2]. A (pseudo-random) sequence of many short pulses is emitted within the time-of-flight of the neutrons to the detector. This drastically enhances the intensity without spoiling the resolution of the instrument. However, for a single neutron it is no more possible to assign the arrival time of the neutron to a time-of flight since it is not known to which pulse it belongs. Additional information is required. At POLDI this is the angular dependence of the arrival times. Plotting the arrival time of the neutrons versus the scattering angle yields a line for each Bragg reflection. The slopes of these lines are proportional to the time-of-flight of the neutrons. The determination of the slope of the Bragg-lines, therefore, allows us to identify the pulse, from which the neutrons came from. And finally, since we know precisely when this pulse was emitted from the copper, we can calculate the time-of-flight of the neutrons.

DESIGN OF THE INSTRUMENT

The instrument design is described in detail in Ref. [3]. The main components are: (i) a fast running chopper with 32 small slits in a pseudo-random distribution, (ii) an elliptical neutron mirror, which images the small slits onto the sample position at a distance of 12 m and (iii) a one-dimensional position sensitive ^{3}He-detector in time-focusing configuration at scattering angles in the range between 75° and 105° with an angular resolution of about 0.08°. Figure 1 shows the sample table the radial collimator and the detector without shielding.

With horizontal and vertical slits in the incident beam and a radial collimator on the secondary side it is possible to define a gauge volume within a large sample. Spatial resolution down to $0.6\times0.6\times1\,mm^3$ is achievable.

Small slits in a fast running chopper in combination with a low divergent beam ensures a high resolution of the instrument. The resolution can be tuned simply by changing

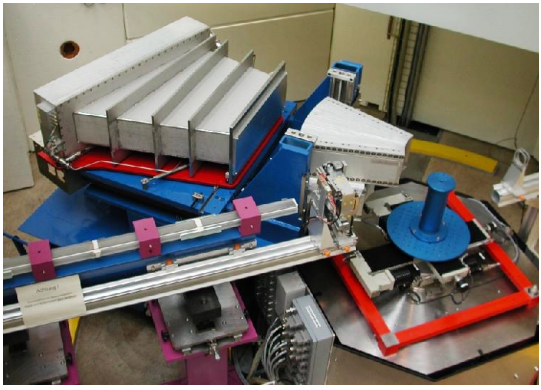

Figure 1: Top view on the POLDI detector, the radial collimator and the sample area. Note that all shieldings have been removed and that the detector is not at its measuring position.

the chopper speed. At highest speed the resolution varies in the range of the achievable lattice spacings from 0.12 % (FWHM) at 3 Å lattice spacing to 0.18 % at 0.8 Å. Therefore the resolution is only weakly dependent on the lattice spacing, an important fact for many material science and residual stress applications.

In Figure 2 the tensile machine for forces up to 30 kN is shown on the sample table of POLDI. This machine is mainly used for material sciences studies.

EXAMPLES FOR MATERIAL SCIENCES STUDIES:

The material science experiments performed on POLDI mainly focused on the line shape analysis and the load transfer of multiphase material under external tensile stress.

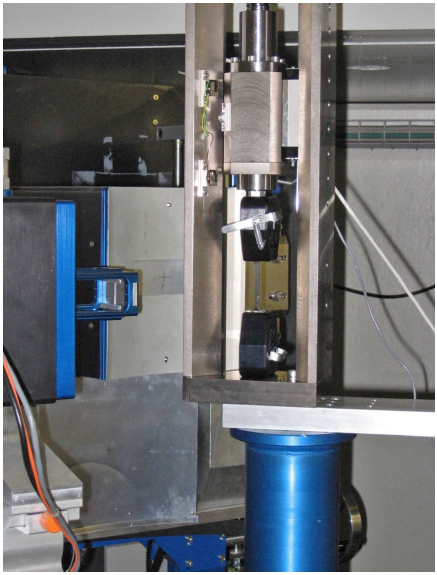

Figure 2: The tensile machine on the POLDI sample table. In the background the radial collimator is visible, on the right site the adjustable slits for the incident beam.

In most superconducting magnets the A15 alloy Nb_3Sn is used as superconducting material. Since this alloy is quite brittle it is embedded in a Cu matrix. The wires in high field magnets have to resist strong Lorentz forces, therefore it is important to optimize their strength and still keep a high critical current density. One method for the production of these wires is a heat treatment of the copper with tubes filled with the parent materials (Nb, Nb_2Sn and Sn). However, the load capacity of such wires is only about 150 MPa. Single wires, consisting of small Nb_3Sn filaments in a Cu matrix have been investigated before and after heat treatment with the tensile machine on POLDI [4]. In Figure 3a the strain of the copper before and after heat treatment is plotted versus the applied load. It shows that after the heat treatment the Cu becomes very soft and looses nearly completely its ability to carry load. In Figure 3b the strain of the A15 Nb_3Sn of the heat treated sample is shown in dependence of the external force. It shows that above 100 MPa there is a load transfer from the soft copper to the brittle Nb_3Sn.

Very high, pulsed, magnetic fields up to 80 T can only be achieved by normal conducting coils. However, the forces on the wires within these coils become very large. Therefore, it is necessary to develop wires with good conductivity and high strength. These requirements fulfill Cu wires which contain Nb nanofilaments. The investigated wires contain more than 9 million Nb filaments with a diameter of about 267 nm each [5]. The dimen-

sions of the channels within the multiscale Cu matrix are between 45 nm for the finest channels and 47 µm for the largest ones. Due to their small grain size the linewidths of the Bragg peaks of the finest channels are significantely broadened. Therefore, it is possible to distinguish between the Copper of these channels and the rest of the copper matrix. This is shown in Figure 4, where the lattice parameter corresponding to the small and broad copper (220) reflection is plotted versus the applied stress. The lattice parameters of the fine copper channels have a stronger dependence on the external force and deviates from linearity at higher stress. Therefore, although the fine Cu channels take more load they remain elastic up to a higher force than the larger channels. The measured yield stress of the fine channels is in agreement with an Orowan–type behaviour, associated with the

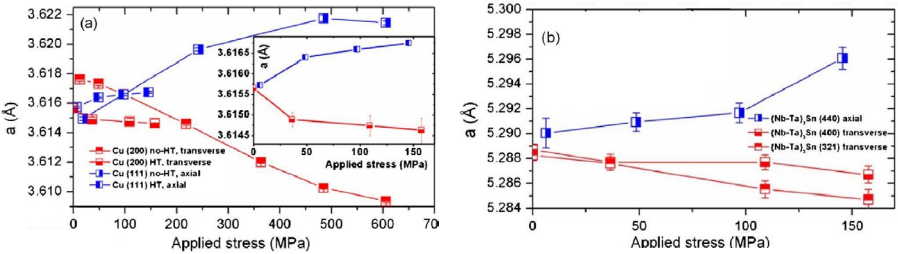

Figure 3: Lattice parameters of Cu and Nb3Sn of a superconducting wire, as determined from fits of single Bragg reflections in dependence of the applied stress. In Figure 3a the results for Cu in axial and transverse direction are shown for the heat treated and non-heat treated wires. The insert shows the result of the heat treated wire in an enlarged scale. The results for the Nb3Sn component of the heat-treated sample are shown in Figure 3b.

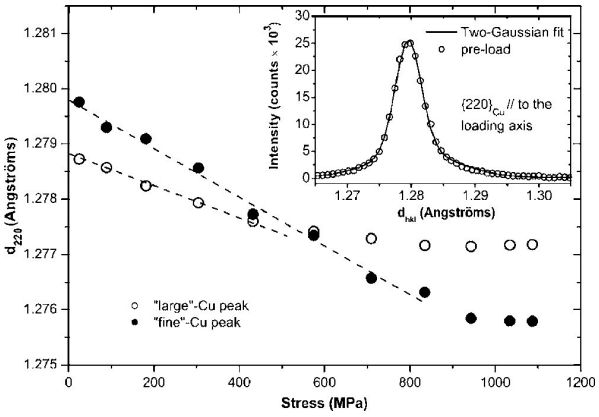

Figure 4: Peak positions of a two-Gaussian fit of the Cu (2 2 0) reflection in transverse direction versus the applied stress. The insert shows the data and the fit in the preloaded state.

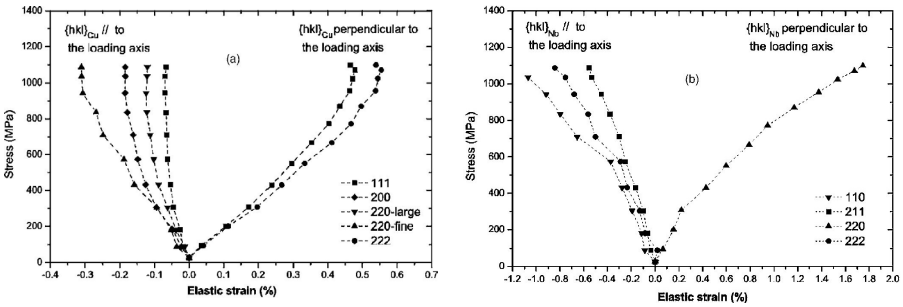

Figure 5: Evolution of the elastic strain of dominant grain families in Cu (Figure 5a) and Nb (Figure 5b) for transverse and axial direction vs. applied tensile stress.

occurrence of a single dislocation regime. In Figure 5 the elastic strains of grains in various directions of Cu and Nb are plotted in dependence on the external force. It shows that above the yield strength of the fine channels there is a load transfer from the copper to the Nb nanofilaments.

EXAMPLES FOR RESIDUAL STRESS DETERMINATION

Residual stress was determined in a pump casing fabricated from a quenched Al alloy, which constitute part of a fuel transmission system in aircrafts [6]. Figure 6 shows a half model of the pump casing. In Figure 7 the corresponding lattice parameter in radial direction of the three strongest reflections along the central line through the thickness of the sample is presented. The data points of the three reflections are on top of each other, which show that the intergranular stresses are negligible. In Figure 8 the stresses determined for the three principle directions are compared with predictions of finite element calculations. There is an excellent agreement between experiment and simulation apart from a small region close to the top surface.

The radial collimators on the secondary side have a quite large distance to the gauge volume of 230 and 420 mm for the 1.5 mm and 4 mm radial collimator respectively. This allows, in combination with the well collimated primary beam to investigate also large samples and keeping still a good spatial resolution. The largest specimen investigated at POLDI up to now were complete railway wheels. The same wheels have been measured at the same positions after various times of usage [7].

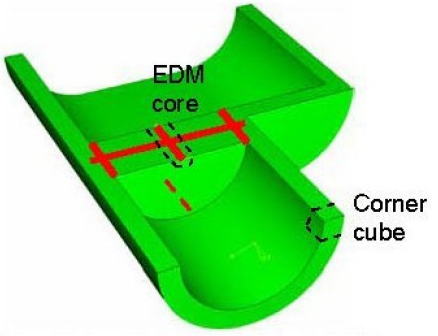

Figure 6: Half model of the pump casing. The lines indicate the lines where the measurements have been done.

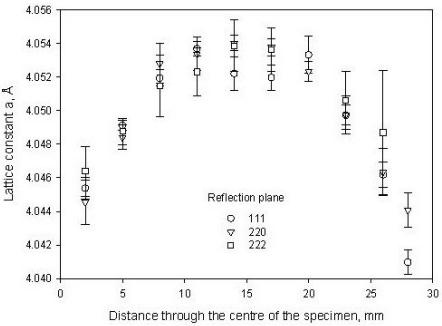

Figure 7: Through thickness scan in radial direction. The lattice parameters, determined from fits to three different reflections are shown in dependence of the measuring position.

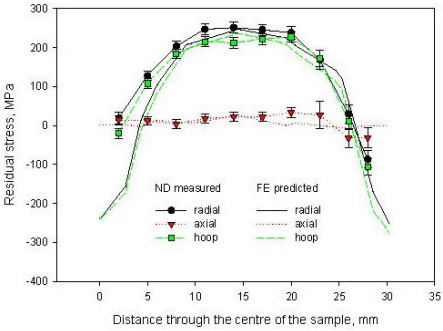

Figure 8: Comparison of the residual stresses determined from the POLDI measurements with finite element calculations of the quenching process.

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SINQ – the First 10 Years: A Scientific Symposium at PSI

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On December 3, 1996 SINQ produced its very first neutrons in a test period of two days. Thereafter in summer 1997 the first experiments under real conditions were made and in spring 1998 the first official call for proposals was launched.

10 years later the Swiss Spallation Neutron Source at the Paul Scherrer Institut already looks back to more than 2200 experiments, 3600 visits of users and approximately 1600 proposals.

The Paul Scherrer Institut celebrated the SINQ jubilee with two events: a scientific symposium on September 21 and an open day for the general public on October 28, "the day of the neutrons".

The SINQ user community and the PSI staff involved in the SINQ project gathered at PSI in September for a dedicated symposium and to take a look back to the first 10 years of SINQ operation.

After the "Welcome" by Kurt Clausen (PSI) Walter Fischer (PSI) reported on the highly interesting period between the late seventies and the early nineties during which the first idea about a neutron source at PSI/SIN was born and later on the realization was undertaken. Albert Furrer (PSI & ETH Zürich) then continued the programme with a description of the construction period from the viewpoint of the neutron scatterers. He gave an overview about the first generation of SINQ instruments and also reminded the audience on SINQ pioneers like Peter Fischer, Peter Böni and the late Willi Bührer, who played an important role for the "day-1"-instruments and the guide system.

Both an external and an internal view was perfectly given by Hans-Rudolf Ott (ETH Zürich). He covered the organisational structure of the SINQ project and of the PSI research department, which is nowadays called NUM ("Solid State Research with Neutrons and Muons"). He also described the process of PSI to shift the focus to the field of solid state physics.

After that it was time to listen to the users of SINQ: Both Ted Forgan (Birmingham) and Kell Mortensen (Copenhagen) described scientific highlights from the fields of "solid state physics" and "soft condensed matter", respectively. They also mentioned their satisfaction with the SINQ facility, the state-of-the-art instrumentation and the support given to the external users by the PSI staff.

The scientific programme did not only cover the history but also the future of SINQ: The last two talks of the colloquy – given by Werner Wagner (PSI) and Joël Mesot (PSI & ETH Zürich) – were dedicated to the latest achievements and future perspectives of the SINQ target development as well as the future instrumentation and scientific strategy, respectively. Werner Wagner recalled the great success of the MEGAPIE project and also described the present activities to develop a more efficient solid target for SINQ, which could bridge the time before MEGAPIE-2 will be realized. Joël Mesot presented not only the ongoing projects to further improve the instruments for neutron scattering and imaging but also showed the impressive publication record and scientific output of the facility and its instruments.

After a guided tour through the SINQ halls the participants finally enjoyed a delicious dinner at the PSI restaurant and used the opportunity for both meeting old friends and to create new contacts for further experiments at SINQ.

Impressions from the banquet on Sept. 21:










Visitor Day at PSI: **October 28, 2007 was the "Day of the Neutrons"**

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NUM department, Paul Scherrer Institut, Villigen

After the great success of the last public visitor day in 2005 the Paul Scherrer Institut again opened its doors and invited the general public to a dedicated "day of the neutrons" on Sunday, October 28, 2007.

The subtitle of the event was *"spies in the micro cosmos"* and was meant to attract the people's attention to the fascinating property of the neutrons to probe the microscopic world and to deliver valuable information about samples from various fields like physics, chemistry, biology and materials science.

More than 3500 visitors came to PSI and were informed about the research with neutrons and the experimental facilities. At six large visitor stations the people were introduced to the technique and the scientific applications of both neutron scattering and imaging:

Station 1 was dedicated to medical applications: Highly interesting and easily understandable for a broad audience Peter Schurtenberger and Anna Stradner from the University of Fribourg reported about their research on the origin of the "grey cataract". The PSI lecture hall was completely filled for each of the three presentations given that day. After each presentation an ophthalmologist – Bruno Blumer from the "Kantonsspital Aarau" – was there to answer medical questions from the audience.

In station 2 the visitors were introduced to the experimental facilities dealing with low temperatures, high pressure or magnetic fields. They could experience how strong magnetic fields can be and what might happen to objects from "every day life" when being cooled to liquid nitrogen temperatures. In a competition they could test their ability to estimate and compare pressures in our daily life.

Another attraction was set up with valuable help from the Universities of Geneva and Neuchatel in connection with the Swiss NCCR MaNEP project ("Materials with Novel Electronic properties", http://www.manep.ch). Several demonstration experiments were exhibited to show the possible future applications of high temperature superconductors. One of the "highlights" was the "Suprasurf", a chair equipped with superconductors levitating over a magnetic railway. The visitors could


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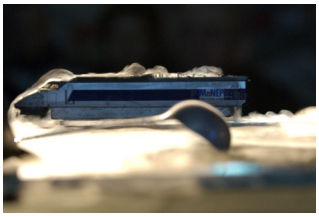
take a tour and were impressed by the experience to be suspended and to glide over the rails without any contact.

Two large multimedia stations then presented the techniques and applications of neutron scattering and imaging: Every 30 minutes experts from PSI gave popular talks and presented manifold examples from materials science, cultural heritage, archaeology on the one hand and superconductivity on the other. In particular it was explained how neutrons can contribute to solve the "mystery" of high-temperature superconductivity. Those presentations were given inside the SINQ halls, which were darkened and illuminated in a spectacular manner for this special event.

The scientific programme was accompanied by various further attractions: The PSI visitor centre "Forum, http://www.psiforum.ch" was open and showed its exhibition. The team from the PSI restaurant OASE spoiled the visitors again with delicious catering. In particular the people enjoyed the ice cream produced by liquid-N_2.

Many thanks to all the staff involved who made this event a huge success both for the interested visitors and for PSI. The institute was able to present its neutron activities to a broad public audience. The generous support from the universities Geneva and Neuchatel and from the MaNEP project is gratefully acknowledged as well.



Announcements

SGN/SSDN Members

The Swiss Neutron Scattering Society welcomes the following new members:

Francisco Cuesta-Soto, Valencia, Spain
Raul Erhan, Dubna, Russia

Presently the SGN has 204 members. Online registration for new members of our society is available from the SGN website: http://sgn.web.psi.ch

SINQ Call for Proposals

The next DEADLINE for the submission of beam time requests for the Swiss spallation neutron source "SINQ" (http://sinq.web.psi.ch) will be:

January 31, 2008

This is a special call for proposals for the beam time period I/08 between 01/05/2008 and 31/08/2008 and from then onwards (long-term proposals) only for the following instruments:

TASP, RITA-II, SANS-II, POLDI, TRICS, NEUTRA, ICON

The next regular deadline for all SINQ instruments will be as usual May 15, 2008.

Registration of Publications

You are kindly asked to register your SINQ related publications within the PSI Digital User Office DUO: https://duo.psi.ch. In particular we need the information about the 2007 publications for the annual reports. Please use the link "publications" from the DUO main menu and follow the online instructions. The DUO publication tool is easy to use and self-explaining but please don't hesitate to contact us if anything remains unclear: sinq@psi.ch. You can use your DUO publication records as a reference in your new proposals.

Erasmus Mundus Program MaMaSELF

MaMaSELF is a one year European Master program (2nd Master year) in Materials Science, which aims to teach the application of "Large Scale Facilities" for the characterization and development of materials. Details on the program are given at http://etudes.univ-rennes1.fr/mamaself/english (please note: Switzerland is counted as non EU-member. The deadline for Swiss applicants is therefore Feb 15, 2008. Swiss applicants can apply for a full grant of 21'000 Euro for the one year course).

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".

We are pleased to announce the International Summer School:

Structure Determination from Powder Diffraction Data

A Hands-on Workshop on X-rays, Synchrotron Radiation and Neutron Diffraction Techniques

The School is jointly organized by the Paul Scherrer Institute (PSI), the Italian Crystallographic Association (AIC) and the Swiss Crystallographic Society (SCCr/SGK).

Where: Paul Scherrer Institute
5232 Villigen PSI – Switzerland
(near Zurich)

When: June 18th - 22nd , 2008

What's new: Hands-on on structure determination from powder diffraction data including data collection at the Swiss synchrotron facility located at PSI and hands-on tutorials on several structural solution and refinement programs (provisional list: EXPO, TOPAS, FullProf, FOX)

Who should come: The School is open to anybody, but the total number of participants is limited to 40 to guarantee a high teacher-to-student ratio. Attendance from emerging Countries, including East Europe, Middle East and Africa is strongly encouraged and special grants will be devoted to attendees from such areas.

Additional information is available on: http://user.web.psi.ch/powder08/

7th PSI Summer School on Condensed Matter Research

August 16–22, 2008

Probing the Nanometer Scale with Neutrons, Photons and Muons

The properties of a material may be dramatically altered either when one or more of its spatial **dimensions are reduced to the nanometer scale or within nanometer distances** from an interface to another material with very different properties. The latter proximity effect may lead to very **strong coupling between properties such as magnetism, resistivity, superconductivity, ferroelectricity,** etc. In this school we will show how **neutrons, synchrotron X-rays and muons** can be used to probe these materials and detect **new phenomena on the nm scale. Various techniques based on the use of neutrons, muons and photons** (powder diffraction, small angle scattering, reflectometry, muon spin rotation/relaxation, real space imaging and X-ray circular dichroism) will be introduced and **examples from the fields of superconductivity, magnetism, ferroelectricity, material science, food science and soft matter science** will be presented.

The school is addressed mainly to the education of PhD and postdoctoral students without prior knowledge of neutron, X-ray and muon techniques. It is fully open to the national and non-national public and the language of the school is English.

More information, registration etc:
http://num.web.psi.ch/zuoz2008/

Conferences and Workshops 2008

JANUARY

Magnetic Structure Determination Workshop 2008
January 14–17, 2008, The Cosener's House, Abingdon, United Kingdom

Winter School in 3D Light and Electron Microscopy
January 13–18, 2008, ETH Zurich, Switzerland

ISNS 2008: International Symposium on Neutron Scattering
January 15–18, 2008, Mumbai, India

SOLEIL Users Meeting 2008
January 17–18, 2008, Ecole Polytechnique – Palaiseau, France

2nd Symposium Hydrogen & Energy
January 21–25, 2008, Braunwald, Switzerland

2nd European XFEL Users' Meeting
January 22–23, 2008, DESY, Hamburg, Germany

APNFM2008 – International Conference Advanced Processing of Novel Functional Materials
January 23–25, 2008, Dresden, Germany

FEBRUARY

1st ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite
February 11–15, 2008, Grenoble, France

HERCULES 2008
February 17– March 20, 2008, Grenoble, France

72th Annual Meeting of the German Physical Society DPG
February 25–29, 2008, Berlin, Germany

PD2DD: Workshop on Powder Diffraction with 2-Dimensional Detectors
February 26–27, 2008, Grenoble, France

MARCH

16th Annual Meeting of the German Society for Crystallography
March 3–6, 2008, Erlangen, Germany

International J-PARC Symposium on Pulsed Neutron and Muon Sciences
March 5–8, 2008, Mito, Japan

29th Berlin School on Neutron Scattering
March 3–17, 2008, HMI Berlin, Germany

TMS 2008: Linking Science and Technology for Global Solutions
March 9–13, 2008, New Orleans, Louisiana, USA

March Meeting of the Swiss Physical Society including a MaNEP Session
March 26–27, 2008, Geneva, Switzerland

APRIL

Summer School on Mathematical and Theoretical Crystallography
April 27 – May 3, 2008, Gargnano, Garda Lake, Italy

MAY

MaMaSELF workshop
May 7–9, 2008, Rigi, Switzerland

ACNS 2008: American Conference on Neutron Scattering
May 11–15, 2008, ILL, Santa Fe, NM, USA

HSC7: Synchrotron Radiation and Neutrons for High Pressure Studies
May 18–24, 2008, Grenoble, France

Surfaces and Interfaces in Soft Matter and Biology: the impact and future of neutron reflectivity - A Symposium in Honor of Robert K. Thomas
May 21–23, 2008, ILL, Grenoble, France

16emes Journees de la Diffusion Neutronique
May 23–30, 2008, Albe, Alsace, France

2007 Annual Meeting of the American Crystallographic Society
May 31 – June 5, 2008, Knoxville, USA

JUNE

European Summer School on Scattering Methods Apllied to Soft Condensed Matter
June 7–14, 2008, Bombannes, France

ICQ10: 10th International Conference on Quasicrystals
June 9–14, 2008, Zurich, Switzerland

5th International Conference on New Developments in Photodetection
June 15–20, 2008, Aix-les-Bains, France

JULY

SXNS 10: International Conference on Surface X-Ray and Neutron Scattering
July 2–5, 2008, LLB Saclay, France

μSR 2008: 11th International Conference on Muon Spin Rotation, Relaxation, and Resonance
July 21–25, 2008, Tsukuba, Japan

STRIPES 08: 6th International Conference of the "Stripes and High-Tc Superconductivity" Series
July 26 – August 1, Erice, Sicily, Italy

AUGUST

7th PSI Summer School on Condensed Matter Research
August 16–22, 2008, Zuoz, Switzerland

IUCr 2008: XXI Congress of the International Union of Crystallography
August 23–31, 2008, Osaka, Japan

SEPTEMBER

ISBB 2008: 16th International Symposium on Boron, Borides and Related Materials
September 7–12, 2008, Matsue, Shimane, Japan

NOVEMBER

ICTF 14: 14th International Conference on Thin Films
November 17–20, 2008, Ghent, Belgium, Belgium

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

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