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Editorial

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Cover illustration

The participants of the first 'Swiss-Danish Workshop on Neutron Scattering' at PSI on November 16/17, 2001 (see contribution in this issue).

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The SGN/SSDN President's Page

Dear members,

the annual meeting of our society on November 16 at the PSI has provided us with an assessment of the scientific activities of the neutron scattering community. A large part off the meeting was devoted to a discussion of the preliminary version of the strategy paper on the 'Status und Zukunft der Forschung mit Neutronen in der Schweiz'. The aim of the paper has been to identify the 'status-quo' of the research with neutrons in Switzerland and the status and usage of the most important European neutron sources. Furthermore it provides the necessary input for a sound analysis of future developments in the field of neutron scattering from the Swiss point of view, and delivers recommendations for the future Swiss participation at ILL and ESS.

Based on the detailed investigation of the status quo of the research activities in the most important scientific domains where neutron scattering plays an essential role it has once again become clear that Switzerland indeed has a very active neutron scattering community. However, it has also become clear that the activities of the Swiss users is concentrated on relatively few research areas where neutron scattering has traditionally been important in Switzerland (solid state physics, materials science, crystallography). Other areas such as biology or soft matter, that internationally are important groups in the neutron scattering community, are either represented marginally or currently in a stage of being developed only. Nevertheless the detailed survey conducted for the strategy report has shown that the interest in these areas is increasing and that SINQ has a considerable catalytic effect. This may be further enhanced through the new collaboration between the PSI and Risø, where an established and very active soft matter research activity exists. In this respect the Swiss-Danish workshop on the two topics „strongly correlated electron systems“ and „soft condensed matter“ has in fact been a very encouraging first milestone towards a fruitful and intense collaboration between these two communities. Moreover, if a next generation (European Spallation Source, ESS) will be built, there is evidently an enormous growth potential in these domains.

This brings me finally to an attempt to look into the (hopefully) bright future of neutron scattering in Switzerland. It has become clear from the strategy paper that SINQ is and will remain the important home base of the Swiss neutron scattering community. However, it is also clear that this requires that SINQ remains a high priority project within the PSI, and that the PSI continues to invest into the future development of SINQ.

As a second important point it has clearly been demonstrated that there continues to be a strong demand for neutron beam time at the ILL. From our point of view we should therefore strongly urge that current contract between Switzerland and the ILL should be kept running at least for the next 10 years. Moreover, it will be absolutely necessary to participate in a European third generation neutron source. The ESS will be the source of choice, and a strong usage through Swiss groups can undoubtedly be predicted. We should therefore strongly support this project and communicate our support to the relevant organisations. One way of expressing our support could be by participating in large numbers at the ESS presentation days on May 15-17 in 2002. During these days it is planned to present the ESS to the European public, the media, the politician and high level civil servants in the old parliament building in Bonn. Around this meeting, ENSA decided to place as many satellite events as possible involving the different European user communities. As it looks by now, the different European networks related to neutron scattering will have their meetings in Bonn. There will also be meetings of the technical groups of ESS as well as user meetings, associated with the neutron facilities supported by the European large facility access program. In addition, user meetings of as many national European neutron societies as possible would be extremely important as a clear sign of support for this important project. At the moment there is for example a firm commitment to have a German user meeting, which will involve typically 200 persons. During our general assembly the participants agreed that the annual meeting 2002 of the SGN/SSDN should be held in Bonn during the ESS-meeting in order to clearly demonstrate the support of Swiss neutron scattering community for the ESS project. I thus strongly urge all society members to support this event and in particular encourage your students and young collaborators to actively participate and present their results. There will be considerable financial support for young scientists in order to allow them to participate. I believe that this is indeed an important opportunity to demonstrate our interest in the development of a third generation neutron source in Europe that will help us to go far beyond the current limits and work on the scientific problems of the future.

Peter Schurtenberger

Minutes of the SGN/SSDN General Assembly on 16/11/2001

Locality	:	PSI Villigen, Auditorium WHGA/001
Start	:	10:34
End	:	12:18
Participants	:	28 members of the society, 4 non-members

1. Welcome

The president of the SGN/SSDN, Prof. Peter Schurtenberger welcomes the participants to the general assembly 2001. Especially he welcomes the honorary member, Prof. W. Hälg.

2. Minutes of the General Assembly 2000

The minutes of the General Assembly of the SGN/SSDN from Oct 5, 2000 published in Swiss Neutron News 18 (Dec 2000) are accepted without objections.

3. Annual Report of the Chairman (P. Schurtenberger)

The president reports on the activities of the SGN/SSDN in the year 2001:

a) The main activity in 2001 was and still is the preparation of the strategy paper 'Forschung mit Neutronen in der Schweiz – eine Strategie für die nächsten 15 Jahre'. The assembly will deal with that in detail in topic 8.

b) Another activity in 2001 was the implementation of a new Internet website of the society (http://sgn.web.psi.ch). Peter Schurtenberger shows the new pages to the audience.

c) Finally he reports on the member status of the society: in the running year seven new members entered the society, 2 members left the SGN/SSDN. Presently the society has 200 members.

4. Report of the Treasurer (S. Janssen)

Balance 2000:

Property SGN/SSDN 01/01/2000 : **SFr 2.420,10**

	receipts [SFr]	expenditures [SFr]
member-fees (cash-box)	240,-	
member-fees (postcheque-account)	845,-	
donations	30,-	
advertisements (Swiss Neutron News)	200,-	
interests	4,15	
welcome reception Zuoz 2000		455,-
fees postcheque-account		59,40
Total	1.319,15	514,40
Receipts 2000	**SFr 804,75**	
Property SGN/SSDN 31/12/2000	**SFr 3.224,85**	

	Assets [SFr]	Liabilities [SFr]
postcheque-account	2722,80	
cash-box	502,05	
Property SGN/SSDN 31/12/2000	**3224,85**	

5. Report of the Auditors

Both Auditors (W. Fischer, P. Schobinger) have checked the balance 2000. They accepted it without any objections. The participants conclude therefore the release of the SGN/SSDN board.

6. Budget 2001

The treasurer presents the following proposal for the budget 2001:

	Receipts [SFr]	Expenditures [SFr]
member fees	1200,-	
interests	5,-	
welcome reception CH/DK workshop		350,-
fees postcheque-account		60,-
Total	1.205,-	410,-
Receipts 2001	**795,-**	

The participants accept the budget proposal unanimously.

7. News from Neutron Sources and Neutron Source Projects

a) ILL (H. Güdel)

- Colin Carlile has replaced Dirk Dubbers as the new ILL director. From spring 2002 Werner Press will be the German ILL-director.
- An increase of the ILL budget of 11% is foreseen. Generally it has been recognized that also few investments cause a strong improvement of performance which means a large ‘return of investments’.
- The ILL Millennium programme is on its way. The ILL ‘road map’ foresees a lifetime of the institute of another 15 years.
- The Swiss financial contribution to ILL is 3.5%. The Swiss usage dropped slightly from 4.5% in former years down to 3.5%. The government is willing to prolong the contract but it is still a matter of negotiations if the 11% upgrade of the annual budget are also paid by Switzerland.

b) SINQ (S. Janssen)

- Presently 9 instruments are in user operation: HRPT, TriCS, DMC, RITA-II, TASP, FOCUS, SANS, AMOR, and TOPSI out of which one (TOPSI) is scheduled informally. RITA-II is part of the PSI-Risø, FOCUS of the PSI-Saarbrücken cooperation. The strain scanner POLDI will be scheduled for the first time in the next SINQ-cycle I/02.
- News on certain instruments:
  - AMOR : 2d-detector, TOF-mode, polarised neutrons available from I/02 onwards
  - RITA-II : first instrument of PSI-Risø cooperation, operational
  - FOCUS : MICA-monochromator in I/02 available (ΔE_{min}=8μeV)
  - TriCS : from I/02 all three 2d-detectors and software available
  - POLDI : strain scanner, will be scheduled I /02
  - SANS : new detector electronics works well
- Statistics:

  The following average numbers per year have been evaluated for the period 1999-2001: number of proposals:100, number of visits: 180, number of users: 98, Swiss share of beamtime: 53%. In average 67% of the requested beamtime was allocated. 'Magnetism' holds a share of about 1/3 of the instrument days followed by 'Strongly Correlated Electron Systems', 'Superconductivity', 'Structure', and 'Materials Science' with ca. 12-15%.
- The PSI-Risø cooperation is proceeding well. The first instrument (RITA-II) is already in user operation, the SANS-instrument will follow in spring/summer 2002. The Swiss-Danish workshop on Neutron Scattering should serve to strengthen also the scientific cooperation between both user communities.
- From 2002 onwards SINQ will have access to European funds within the framework program 'FP5'. This money will be totally available for the users e.g. in terms of funding travel expenses.

c) European Spallation Source, ESS (A. Furrer)

- The three largest European countries (UK, DE, FR) face difficulties in funding the ESS-project. Since a new ESS council and scientific advisory committee is installed the project gains new activity.
- A recent workshop in Engelberg/CH – partly organised by the PSI – came out with a document entitled ‘Scientific Trends in Condensed Matter Research and Instrumentation Opportunities at ESS’ that condenses trends in the main research areas as well as instrumental needs at ESS. Copies of the document can be obtained from A. Furrer.
- In 2003 a proposal should be completed that can be handed over to the governments and funding agencies.
- An important milestone on that way will be an ESS-meeting in Bonn/DE (15/05-17/05/02) during which the ESS-project should be presented to the public. It is foreseen to assemble many European user communities there with their national assemblies, user meetings etc. The SGN/SSDN should identify how we will contribute to that event (see topic 10).

8. Strategy-paper on the ‘Status und Zukunft der Forschung mit Neutronen in der Schweiz’

Peter Schurtenberger reports on the strategy paper whose preliminary draft version has been distributed electronically among the SGN/SSDN members. Further hardcopies are available during the meeting. The draft version can also be downloaded from the SGN-webpages. Peter Schurtenberger thanks all contributors for their work.

The aim of the paper is to identify the ‘status-quo’ of the research with neutrons in Switzerland and the status and usage of the most important European neutron sources. Additionally it should analyse future developments in the field of neutron scattering from the Swiss point of view. The paper should deliver recommendations for the future Swiss participation at ILL and ESS. Some of the main statements are:

- SINQ : SINQ is of utmost importance as the home base of Swiss neutron scattering. It is also absolutely necessary to further upgrade SINQ. PSI should treat it also in the future as a high priority project.
- ILL : The Swiss community still has a great need for beamtime at ILL.
- ESS : A Swiss participation in the ESS-project is strongly recommended.

- ISIS : There is only a low Swiss request for beamtime at ISIS. This will even decrease further if the ESS would be realized.

Additionally a Swiss participation in AUSTRON is only recommended if the ESS will not be realized.

The assembly discusses the draft version and finally accepts it unanimously with some minor revisions:

- The final sentence on page 49 (‘Befürwortung der ESS’) is not strong enough.
- It should be made clear that also during the project phase a Swiss participation is essential.
- The title should refer only to Neutron Scattering since there is no contribution from the non-diffractive user community in Switzerland: ‘Status und Zukunft der Neutronenstreuung in der Schweiz…’
- The statistical data of the SINQ-chapter (3.1) should be more detailed and adapted to the style of the ILL data.
- The data in chapter 2 (Swiss usage of neutron sources) refers to 1995. It should be stated that there is no big change on that since then.

Further comments and minor revisions can be send per e-mail up to Nov 30 to: ‘peter.schurtenberger@unifr.ch’.

9. Election of the Swiss Delegate in the ILL subcommittee 7

Since 1994 Switzerland has a representative in the ILL College 7 ‘Materials Science, Surfaces, Spectroscopy’ (94-97: G. Kostorz, 98-01: B. Schönfeld, both ETH Zürich). Peter Schurtenberger thanks Bernd Schönfeld for his work in the committee which he has to leave now after 4 years and mentions that either G. Kostorz or P. Allenspach (LNS) would like to candidate for the job.

G. Kostorz explains that he would only be willing to do so if no other candidate could be found. In that case he would offer his expertise in the respective field. Hence P. Allenspach is the only candidate and is elected by the participants of the assembly unanimously. P. Schurtenberger therefore will propose P. Allenspach as the new Swiss representative in college 7 to the ‘Bundesamt für Bildung und Wissenschaft’.

10. Acivities of the SGN/SSDN 2002

Zuoz 2002 (10/08-17/08):

W. Fischer explains that from 2002 onwards the character of the summer school will be changed. It will no longer be restricted to neutron scattering only but will also include generally ‘techniques available on large scale facilities’. It will be organized every second year from now on and the 2002 school will be on the topic ‘Magnetism’. The main organisation will be done by the ‘FUN’ department at PSI.

ESS-presentation in Bonn (15/05-17/05):

The national neutron user communities are strongly encouraged to participate in the ESS-presentation in Bonn. The participants discuss in which way the SGN/SSDN could contribute to that meeting. They agree that the annual meeting 2002 of the SGN/SSDN should be held in Bonn during the ESS-meeting in order to clearly demonstrate the support of the Swiss neutron scattering community for the ESS project. It will be possible to support especially the participation of young scientists.

The SGN/SSDN will furthermore ask the PSI to consider organizing the SINQ user meeting also during the ESS-event in Bonn.

Furthermore, in view of the enormous number of scientific meetings it is felt that the annual meeting of the SGN/SSDN is too close to that of the SINQ user meeting which is traditionally helt in January. The assembly therefore concludes that from 2003 onwards the annual meeting of the SGN/SSDN should be generally combined with the SINQ user meeting.

11. Varia

H. Grimmer announces a workshop on ‘Neutron and Synchroton X-Ray Scattering in Condensed Matter Research’ which will be organised as a satellite conference of the IUCr-meeting 2002. The workshop will take place at PSI from 04-06/08/2002.

S. Janssen, Secretary

Site Symmetry and NH_3 Dynamics in $Mg(NH_3)_2Cl_2$ Studied by Quasielastic Incoherent and Elastic Coherent Neutron Scattering

F. Altorfer
Laboratory for Neutron Scattering, ETHZ & PSI

1. Introduction

Neutron time-of-flight spectroscopy is well suited to probing the reorientational dynamics of atoms and molecules in condensed material, especially those with hydrogen motions due to the large incoherent cross section [1]. We report on studies to investigate the temperature dependence of the NH_3 dynamics in $Mg(NH_3)_2Cl_2$ by means of incoherent quasielastic neutron scattering in the temperature range from 15 to 300 K.

2. Experimental

Sample preparation procedures are described in [2]. Neutron time-of-flight measurements were carried out on the FOCUS spectrometer at SINQ, Paul Scherrer Institute. Due to the temperature dependent wide range of broadening (and to observe this broadening over a wide Q-range in order to distinguish between possible jump diffusion models such as jumps by 120 degrees (3-fold symmetry) or 90 degrees (4-fold symmetry) , see below) we performed scans at two neutron energies: 4.27 meV and 20.0 meV for T≥ 150 K in order to adapt FOCUS' resolution to the NH_3 dynamics. The respective elastic energy resolutions were ΔE = 0.138 and 1.63 meV. A detailed description of FOCUS can be found in [3]. The powder samples, always handled under glove box conditions, were encapsulated in thin walled, cylindrical aluminum containers of 2.5 mm diameter. Data sets were collected covering a scattering angle range from 10 to 130 degrees and in the temperature range from 15 to 350 K. The run at 15K was used to determine the instrumental resolution of FOCUS. In order to determine the onset of the order-disorder transition in $Mg(NH_3)_2Cl_2$, we performed a neutron diffraction study using SINQ diffractometer DMC in the temperature range from 15 K to 250 K. The sample was in a cylindrical vanadium container and the incident neutron wavelength was λ=2.56 Å.

3. Structure and order-disorder transition in $Mg(NH_3)_2Cl_2$

Neutron powder diffraction on $Mg(ND_3)_2Cl_2$ [2] revealed uniaxial orientational order-disorder behaviour of the ND_3 groups as a function of temperature. At low temperatures (T = 8 K) $Mg(ND_3)_2Cl_2$ is ordered with respect to the ND_3 groups: They are arranged antiferroelectrically on either side of the chains (see figure 1 right). The symmetry is lowered compared to the situation at ambient temperatures which involves a doubling of the orthorhombic *c* axes: The authors of reference [2] found for $Mg(ND_3)_2Cl_2$: space group *Ibmm*, and lattice parameters of a = 8.1319(3) Å, b = 8.1338(3) Å, c = 7.4410(2) Å

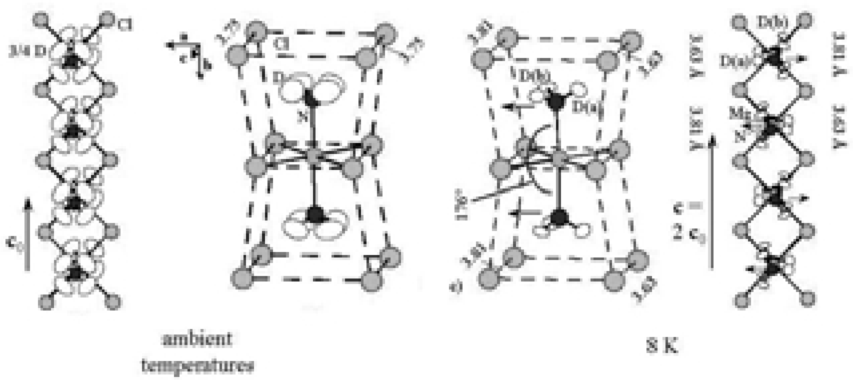

Fig. 1 *High (right) and low (right) temperature structure of $Mg(ND_3)_2Cl_2$. Time average finally leads to the observed distribution of D atoms with four density maxima. The D atom density is well described by a fourfold split position, each D "site" connecting a N with a Cl atom: The c axis corresponds to the direction of the chains. Note that at temperatures higher than 135 K (110 K for $Mg(NH_3)_2Cl_2$) the point symmetry of the N site (C2v) is incompatible with the threefold symmetry of the ND_3 molecule (C3v) that rotates about the N-Cl axis. Pictures taken from reference [2].*

At ambient temperatures the ND_3 groups are disordered with respect to a rotation about the bond Mg N. The D atom density is well described by a fourfold split position, each D "site" connecting an N with an Cl atom: $Mg(ND_3)_2Cl_2$, *Cmmm*, a = 8.1828(6) Å, b = 8.2007(6) Å, c = 3.7543(2) Å, the *c* axis corresponds to the direction of the chains.

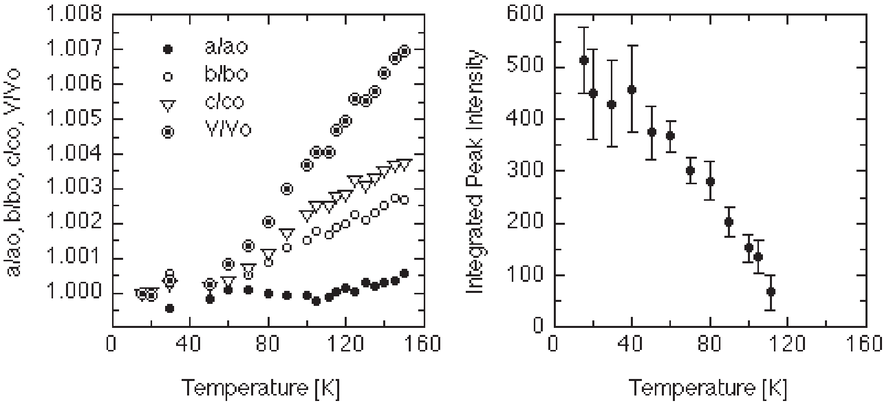

***Fig. 2** (Left): Temperature dependence of normalized (T=10 K) lattice parameters (a/a_0, b/b_0, c/c_0) and unit cell volume V/V_0 in $Mg(NH_3)_2Cl_2$ obtained by neutron diffraction on SINQ's diffractometer DMC. As in the deuterated sample a change of slope in a/a_0 occurs at the order-disorder transition, in $Mg(NH_3)_2Cl_2$ at T=110 K, indicated by the arrow. (Right): The decrease of the integrated intensity of the (103) reflection mirrors the continuous phase transition Ibmm to Cmmm in $Mg(NH_3)_2Cl_2$*

In $Mg(ND_3)_2Cl_2$, the order-disorder transition occurs at 135K. The analysis of the diffraction experiment data on $Mg(NH_3)_2Cl_2$ showed that the intensity of the (103) reflection of the low temperature modification of $Mg(NH_3)_2Cl_2$ vanishes at T=110 K (see figure 2 , right). As in the deuterated sample a change of slope in the normalized lattice parameter a/a_0 (where a_0 at T=10 K) occurs at the order-disorder transition, in $Mg(NH_3)_2Cl_2$ T=110 K (see Fig. 2, left).

4. NH_3 dynamics in $Mg(NH_3)_2Cl_2$

4.1 Model 1: Proton jump between sites separated by 120 degrees (3-fold symmetry)

What is the appropriate model to analyze the quasielastic scattering signal? Since the diffraction data for $Mg(NH_3)_2Cl_2$ shows that the NH_3 molecules have well defined threefold symmetry positions we apply for data sets below T=110 K a model where the three protons of the NH_3 molecule jump between their sites on a circle, separated by 120 degrees. The neutron scattering law $S(Q,\omega)$ for a powder sample, where protons are jumping with a jump rate of τ^{-1} between equivalent sites on a circle is given by

$$S(Q,\omega) = A_0(Q)\delta(\omega) + A_1(Q)\frac{6\tau}{\pi(9+4\omega^2\tau^2)} \qquad (1)$$

with the prefactors $A_0(Q)$ and $A_1(Q)$ as

$$A_0(Q) = \frac{1}{3}\left[1 + 2\frac{\sin(Qr\sqrt{3})}{Qr\sqrt{3}}\right] \tag{2}$$

and

$$A(Q)_1 = \frac{2}{3}\left[1 - \frac{\sin(Qr\sqrt{3})}{Qr\sqrt{3}}\right] \tag{3}$$

Q is the absolute value of the scattering vector, the energy transfer and r the proton distance to the rotation axis. By describing $S(Q,\omega)$ by equation (1), the temperature dependence of the Lorentzian full-width at half maximum (FWHM), $f_w(T)$, is found. The activation energy E_a, the prefactor P and thus the jump rate τ^{-1} are then derived to be

$$\ln\left(f_w(T)\right) = P_0 - \frac{E_a}{kT} \tag{4}$$

As can be seen from Fig. 3, we observed a strong broadening of the elastic line in the time-of-flight data, starting at temperatures $T \geq 85K$. Raw neutron scattering data were grouped into ten data sets, corrected by vanadium runs for detector calibration and empty can runs and then transformed to $S(Q,\omega)$.

We observe an Arrhenius type behavior $\exp(-E_a/kT)$ of the Lorentzian FWHM of the incoherent quasielastic broadening in $Mg(NH_3)_2Cl_2$ over a wide temperature range (see figure 3 (insert bottom)). The analysis of the data leads in terms of the 1-Lorentzian model leads to an activation energy of E_a= 43.2(8) meV and r=0.677(5) Å. The elastic incoherent structure factor (EISF, defined by $A_0(Q)$ in equation (2)) has two major properties: The width of the Lorentzian is independent of the scattering vector Q and the EISF is temperature independent for all Q values. Experimentally determined EISF's for $Mg(NH_3)_2Cl_2$, shown in the top insert of Fig. 3 can be nicely described by the simple jump model and the EISF values at a given Q are fairly independent of temperature.

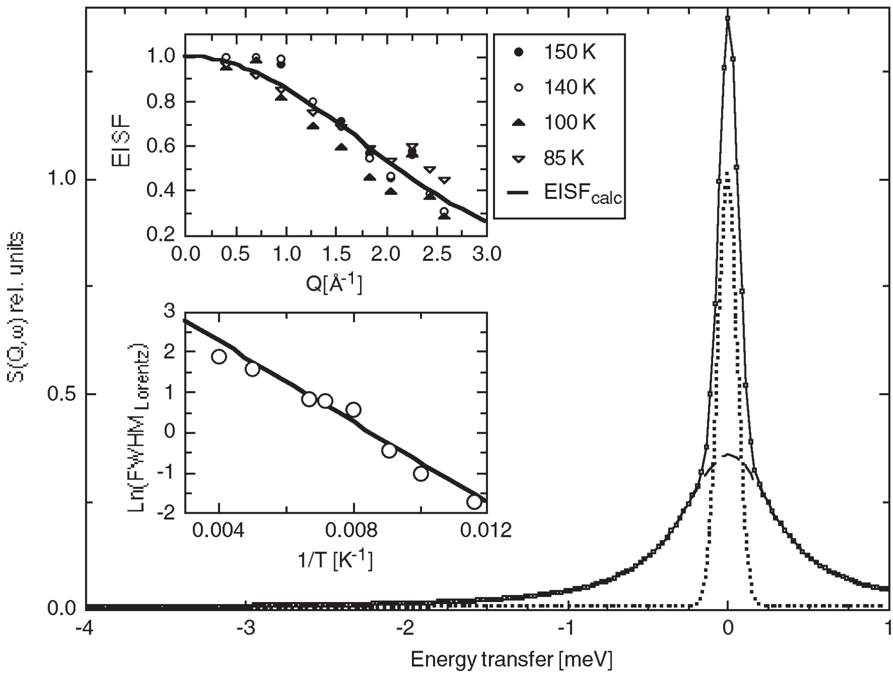

Fig. 3 *Neutron time-of-flight spectrum of $Mg(NH_3)_2Cl_2$ measured at T=110 K, Q=2.565 $Å^{-1}$, E_i = 4.27 meV with Gaussian (dotted) and Lorentzian component (dashed). The instrumental elastic energy resolution is 0.138 meV. Insert (top): Experimentally determined EISF at T=85, 100, 140, 150 K and calculated (line) EISF with r=0.677(5) Å.. Insert (bottom): Temperature dependence of Lorentzian fullwidth at half maximum in $Mg(NH_3)_2Cl_2$ determined by neutron incoherent quasielastic scattering at T=85, 100, 110, 125, 140, 150, 200 and 250 K. The data is well described by an Arrhenius like behavior $ln[fw(T)] = P_0$-Ea/kT) with an activation energy E_a=43.2(8) meV.*

4.2 Model 2: proton jump between sites separated by 90 degrees (4-fold symmetry)

For temperatures higher than 110 K one has also to consider jump diffusion between sites with a four-fold symmetry derived from diffraction data. Now the protons of the NH_3 molecule jump between their sites on a circle, separated by 90 degrees. Note however that this picture is somewhat artificial since the NH_3 molecule simply cannot be accommodated on a four-fold symmetry site. The scattering law thus changes from a one-Lorentzian (see (1)) to a two-Lorentzian and we see from equation (5) that the second Lorentzian has twice the halfwidth of the first.

$$S(Q,\omega) = A_0(Q)\delta(\omega) + A_1(Q)\frac{\tau}{\pi(1+\omega^2\tau^2)} + A_2(Q)\frac{2\tau}{\pi(4+\omega^2\tau^2)} \quad (5)$$

and the prefactors $A_0(Q)$, $A_1(Q)$ and $A_2(Q)$:

$$A_0(Q) = \frac{1}{4}\left[1 + 2\frac{\sin(Qr\sqrt{2})}{Qr\sqrt{2}} + \frac{\sin(2Qr)}{2Qr}\right] \quad (6)$$

$$A_1(Q) = \frac{1}{2}\left[1 - \frac{\sin(2Qr)}{2Qr}\right] \quad (7)$$

$$A_2(Q) = \frac{1}{4}\left[1 - 2\frac{\sin(Qr\sqrt{2})}{Qr\sqrt{2}} + \frac{\sin(2Qr)}{2Qr}\right] \quad (8)$$

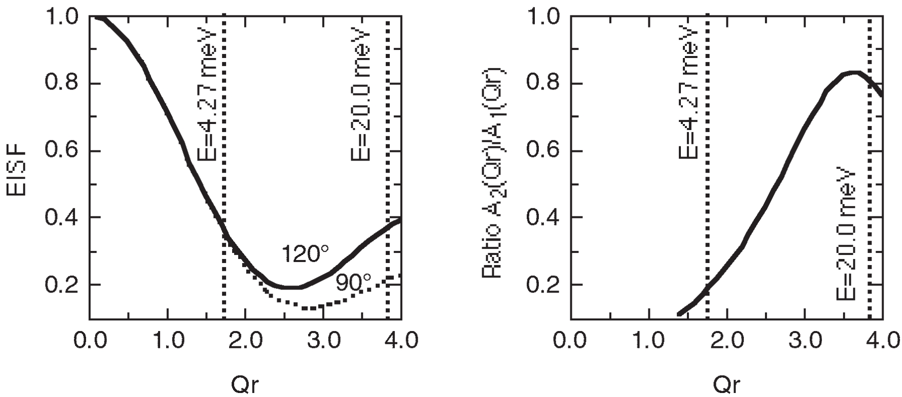

Fig. 4. *(Left): Elastic incoherent structure factors for proton jumps over four sites (dotted, 90°) and three sites (full line, 120°) start to differ from each other for (Qr >2), thus requiring experiments at larger Qr values. (Right): Ratio of structure factors for the two Lorentzian components A_1 and A_2 (equations (7) & (8)). Qr limits for scans with incident neutron energies of 4.27 meV and 20.0 meV are indicated.*

Figure 4 demonstrates the differences between the two models. Firstly, a notable difference in EISF occurs for Qr values higher than 2, so that the data taken with higher resolution at incident neutron energy of 4.27 meV with a maximum Qr of 1.7 Å cannot be conclusive to support either model. That is why data was also taken at 20.0 meV to extend the Qr range (see figure 4, left). Secondly, the weight of the second Lorentzian (equation (8)) is a function of scattering vector Q and once again the data taken at E_i=4.27 meV just barely reach the area where any signature of the second Lorentzian could be observed (see figure 4, right). The contribution of the second Lorentzian should be therefore be best visible at Qr values of approximatively 3.6 where the ratio $A_2(Q)/A_1(Q)$ reaches its maximum of 0.829.

However, the inspection of the data taken at T=150 K, thus 40 K higher than the occurrence of the phase transition showed no indication of this second component. Also the analysis in terms of EISF gave no support for jumps between 4 sites. Figure 5 shows the measured EISF at T=150 K and Q> 2.65 $Å^{-1}$ (Qr>1.55). Although the agreement with the calculated EISF from model 1 (jumps between sites separated by 120°) is not perfect, is much better compared to the predictions derived from model 2 (dotted line).

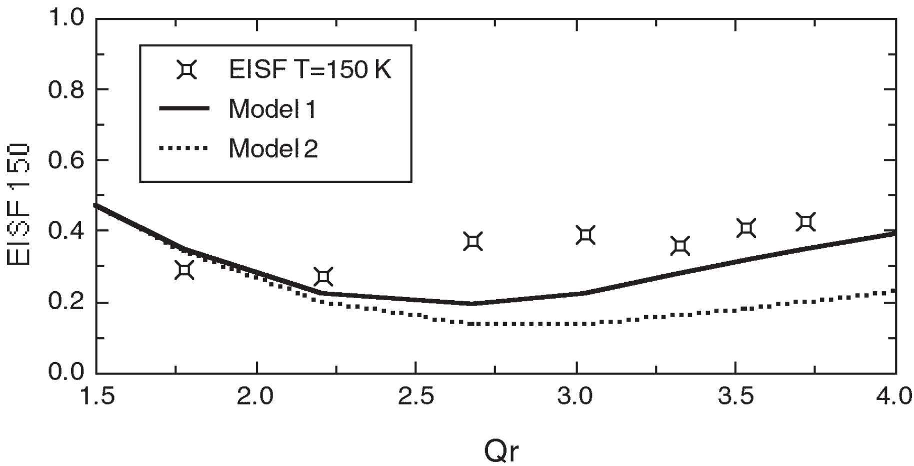

Fig. 5: *Experimentally determined EISF for $Mg(NH_3)_2Cl_2$ using 20.0 meV neutrons at T=150 K. EISF for jumps between sites separated by 120° (Solid line) and EISF for jumps between sites separated by 90° (dotted line).*

Acknowledgements

Contributions by Dr. A. Leineweber, Dr. S. Janssen, Dr. L. Keller are gratefully acknowledged.

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[1] M. Bée, Quasielastic Neutron Scattering, Adam Hilger (1988)

[2] A. Leineweber et al., Jour. of Solid State Chemistry 156 487-499 (2001)

[3] S. Janssen et al., Physica B, 276-278 89-89 (2000)

Design and Present Status of the SINQ Strain Scanning Diffractometer POLDI

U. Stuhr and H. Spitzer
Paul Scherrer Institut, CH-5232 Villigen PSI

Introduction

The new neutron diffractometer POLDI for residual stress measurements at the continuous spallation source SINQ will enter operation in 2002. The main requirements for a strain field diffractometer are high resolution, maximum intensity achievable and the possibility to define a small gauge volume within the sample. This last point implies that the scattering angle should be close to 90°. In order to best meet these requirements, a novel concept of a time-of-flight diffractometer, a so-called multiple pulse-overlap-diffractometer, was used. It combines some of the advantages of angular-disperse (constant-wavelength-), Fourier- and conventional (single-pulse) time-of-flight diffractometers.

The requirements for a strain field diffractometer can be met with a two-axis diffractometer, which is in general most suitable with a continuous neutron source. However, there are some advantages of a tof-diffractometer, the most important is that a whole diffraction pattern can be collected at any scattering angle. Therefore, although the scattering angle is restricted to a small region near 90°, we obtain all structure information of the sample. This is of special importance when there are two or more phases in the investigated gauge volume.

At present two different types of time-of-flight (tof) diffractometers are used for strain scanning. The conventional tof-diffractometers use separate pulses. For each neutron, its wavelength is determined from the time between the pulse of the source or chopper opening, and its detection. For an unambiguous determination of the time of flight and the neutron wavelength, frame overlap is avoided, i.e. the time between successive pulses is chosen in a way that the fastest neutrons cannot catch up with the slowest ones of the previous pulse. Hence, the minimum time between two pulses depends on the length of the flight path and the width of the wavelength band; typical times are in the order of 20ms. This type of diffractometer is mainly used with short-pulsed neutron sources.

The reverse time of flight- or Fourier-diffractometer [1] is based on an entirely different concept. The chopper opening and closing times are the same. Therefore, a detected neutron may have originated from several hundreds of different pulses. Only a combination of many spectra, measured with a variety of frequencies, allows the calculation of the desired wavelength-spectrum.

About a decade ago J. K. Cockcroft and G. J. Kearley proposed a pulse-overlap diffractometer [2] for structure analysis applications. In comparison to a conventional tof-diffractometer, a pulse-overlap diffractometer has much shorter time intervals between the neutron pulses and neutrons of several different pulses may arrive the detector at the same time. The angle dependence of the tof-spectra is used as extra parameter for the analysis of the data. The main advantages of a pulse overlap diffractometer are that it allows (i) to optimise the conflicting quantities of contrast and intensity, of the measured spectra and (ii) to decouple these quantities from the resolution of the instrument. Due to its task of strain-field measurements, which restricts the acceptable angular range, the concept of POLDI is considerably different to that proposed in [2].

The basic concept

The resolution of a tof-diffractometer consists of mainly two components: the uncertainty in the measurement of the time-of-flight t_{flight} from the chopper to the detector and the uncertainty in the determination of the scattering angle 2θ. The uncertainty of the time of flight is, for a given length of the flight path, mainly determined by the width of the neutron pulse. An improvement of the resolution can therefore only be achieved by a shortening of the pulse length. In a conventional tof-diffractometer this has the consequence that the duty cycle and therefore the intensity, decreases. The present instrument concept avoids these restrictions since it allows an overlap of neutron pulses. The resolution can be adjusted by the chopper speed. The duty cycle of the chopper and the range of neutron wavelengths remain unchanged. The intensity is therefore independent of the (time component of the) resolution. Only the number of overlapping Bragg lines increases with higher chopper speed.

Since in a multiple-frame-overlap-diffractometer the arrival time of a neutron does not unambiguously determine the time of flight of the neutron, an additional parameter is needed, which allows the determination of which slit the neutrons came from. This additional quantity is in our case the dependence of the arrival time of the neutrons of a given Bragg reflection on 2θ.

The time of flight of a neutron between chopper and detector is:

$$t_{flight} = \frac{2 \cdot m_n}{\mathrm{h} \cdot Q} \cdot s_{tot}(\theta) \cdot \sin\theta \qquad (1)$$

where $\eta Q = 2\pi\eta / a_{hkl}$ is the momentum transfer of a neutron scattered at a Bragg-reflection with a lattice spacing a_{hkl}, η is Planck's constant, m_n is the neutron mass and s_{tot} is the total length of the flight path of a neutron from the chopper to the detector, which may vary with the scattering angle. In a contour plot of the arrival time of the neutron versus scattering angle each Bragg-reflection is represented by a line. The slopes $dt/d\Theta$ of these lines can be expressed as a function on Q and Θ, or of the time-of-flight and Θ,

$$\frac{dt}{d\theta} = t_{flight} \cdot \left(\cot\theta + \frac{1}{s_{tot}} \cdot \frac{ds_{tot}}{d\theta} \right) \qquad (2)$$

Therefore, if we can determine the slope t_{flight} with sufficient accuracy, we can trace the slit of the chopper that the neutrons came from, and hence determine its wavelength unambiguously.

A lower limit of the time interval between two chopper pulses is therefore given by the precision of the determination of the slope. The optimum value for the duty cycle can be found for example by considering the expected contrast of the spectra [3].

This concept leads to a quite simple layout of the instrument. A sketch of the POLDI-instrument is given in Fig. 1

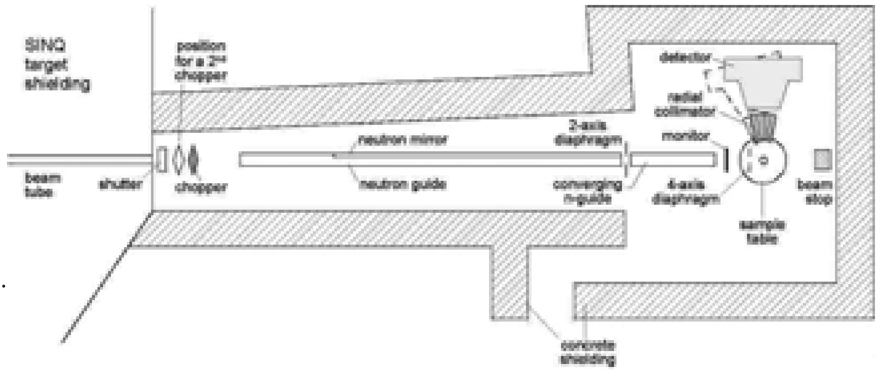

Fig. 1: *Sketch of the POLDI-instrument*

Layout of the main instrument components

<u>Chopper</u>

The disk-chopper has a diameter of 700 mm, a maximum speed of 15000 rpm and 32 slits, each with a width of 4 mm. This yields a minimum pulse width of 8µs (FWHM) and a duty cycle of 5.8%. Since the total length of the flight path is nearly 14 m, the pulse width contributes to the relative uncertainty of the time of flight with $\sim 8.6 \cdot 10^{-4}$, for 2.6 Å neutrons. A photo of the chopper disc is presented in Fig. 2.

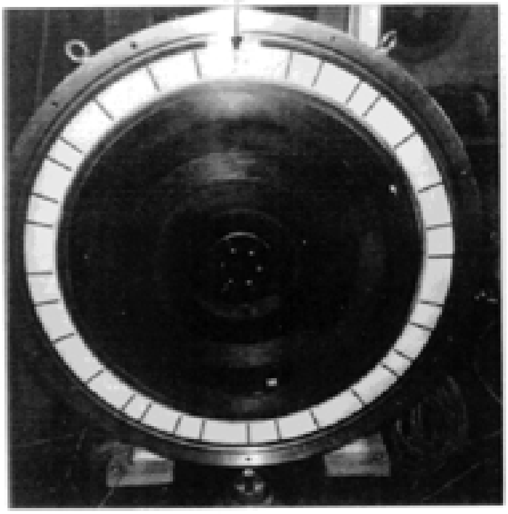

Fig. 2: *Picture of the chopper disk*

Neutron optics

To get short chopper pulses and to reduce the background (fast neutrons and γ-radiation) the width of the beam at the chopper position has to be small. Therefore, the neutron optics between chopper and sample is important in order to minimise losses of neutron density in the phase space. The best way to transmit neutrons with minimum losses is to image the slit at the chopper onto the sample, which is done at POLDI by a neutron mirror with an elliptical surface.

There are some further advantages of such a mirror: (i) the mirror can be much shorter than the chopper-sample distance, therefore there is always enough space to insert equipment and beam manipulation devices like velocity selector, diaphragms etc. (ii) All neutrons are reflected only once, therefore the loss of neutrons loss is minimised and there are only small variations of the reflection angles, allowing an effective suppression of neutrons with wavelengths shorter than a well-defined cut-off wavelength. The latter advantage facilitates the evaluation of the data. Fig. 3 shows the wavelength spectrum at the sample position compared with that at the entrance of the neutron guide. After the mirror a vertical anti-trumpet, as a beam focusing device, further increases the flux at the sample.

Radial collimators are used to define the gauge volume on the secondary side of the diffractometer. At present two radial collimators with spatial resolutions of 1.5 and 4 mm are mounted on the instrument. A third collimator with a resolution of 0.6 mm is planned for end of 2002.

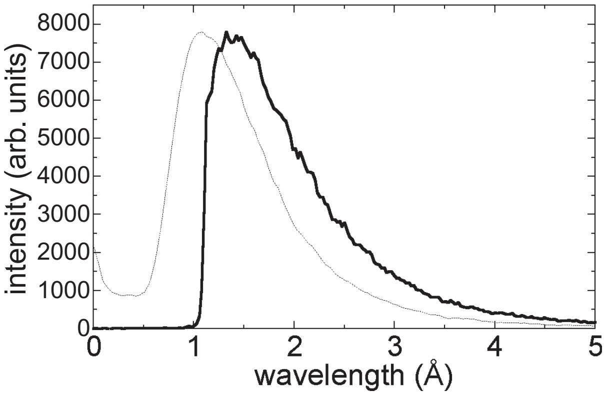

Fig. 3: *Comparison of the wave-length spectra behind the neutron mirror (bold solid line) and at its entrance (thin broken line). Both spectra are normalized to same intensity.*

<u>Detector</u>

A one-dimensional position sensitive banana-type ^{3}He-detector in time focusing geometry is built at the detector group of PSI. The detector collects data in a range of 30°, its centre can be positioned either at 2θ=90° or at 105°. The spatial resolution of the detector is expected to be better than 3 mm. The thickness of the active area of the detector is 40 mm, which corresponds to a time of flight of the neutrons of 20-50 µs. Time focusing is necessary to avoid a time uncertainty of this magnitude, which would spoil the resolution of the instrument. Accordingly to Eq. (2), a time focusing condition (which means that the time-of-flight is independent on scattering angle) is achieved if we choose $1/s \cdot ds_{tot}/d\Theta = cot\Theta$. Since the chopper to sample distance is a constant, $dr = ds_{tot}$, where r is the sample detector distance and the above condition reduces to $1/s \cdot dr/d\Theta = cot\Theta$. However, we cannot choose the orientation of the detector elements separately, we have to fulfil the condition that the position of neighbouring detector elements is perpendicular to the orientation of the given element. This leads to the implicit condition for the shape of the detector

$$const \cdot \frac{s_c}{r(\theta)} \cdot \exp\left(\frac{s_c}{4 \cdot r(\theta)}\right) = \cos\theta \quad (3)$$

where r(Θ) is the distance of the detector element from the sample. Fortunately, the shape of the detector, as described by Eq. (3), can be very well approximated by a circle with a radius of about 3m (for an average distance between sample and detector of 2m) for angles below 130°. Note that the centre of this circle is not at the sample position.

At present the detector is tested and it should be ready for experiments after the shutdown 2001/2002.

More details about the instrument can be found on the POLDI homepage on the internet [4].

Data evaluations

The first step of data analysis will always be the calculation of a diffractogram without any assumptions about the sample or neutron beam properties as the wavelength distribution. This program calculates the intensity for every d-spacing in a given *Q*-range. The only input parameters are the geometrical quantities of the instrument (positions of the slits in the chopper disc, distances and angles), which can be determined with a calibration measurement. The output is a diffraction pattern with the Bragg-peaks at the precise position but with a considerable correlation background and quite large uncertainties in the intensities of the peaks. In Fig. 4 such a correlation diffraction pattern (CDP) calculated from simulation data of Si powder on POLDI is given as an example. The further evaluation depends on the subject of investigation

standard strain scanning: Here the important information is the position and linewidths of the peaks. In this case a fit of the most intense peaks of the CDP is sufficient. A fit of the strongest reflection of the CD in Fig 4 is given in Fig. 5. The advantage of this procedure is that it is fast and that no initial information about the sample is required.

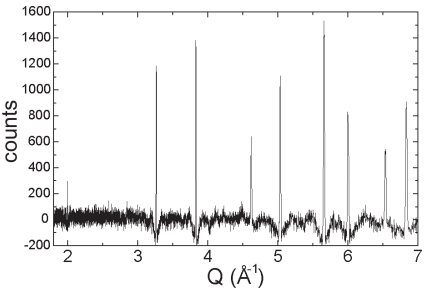

Fig. 4: *Correlation diffraction pattern of simulation results for Si-powder*

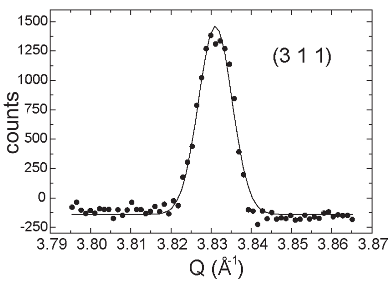

Fig. 5: *Fit of the (3 1 1) Si-reflection at Q=3.83 in Fig. 4*

structure and texture analysis: For this analysis the intensities of the Bragg reflections must be determined which will be done by a Rietveld fit of the complete angle-time plot. Information of the structural phase(s) within the sample as well as good starting parameters of the lattice parameters can be derived from the first CDP. Fig. 6 shows the result of the fit plus residuals of the same data as in Fig. 4. The results of these fits give much more precise information on the intensities of the peaks and, as a consequence, the residuals which determine the statistical fluctuations are much smaller than the correlation background of the CDP.

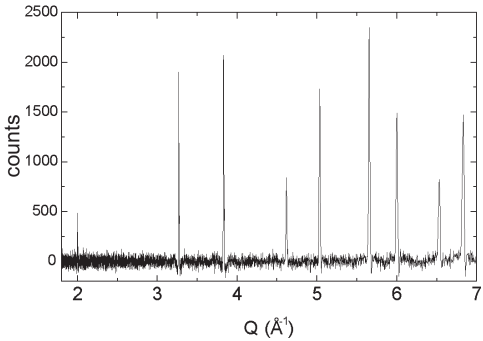

Fig. 6: *Result of a fit plus residuals of the same data as in Fig. 4.*

A 2-D plot of the residuals shows if there are any systematic deviations between the measured and the fitted spectrum. Often strain measurements have to be done in directions of the principle axis of the strain tensor. Significant deviations of the lattice parameter in the angular range of the detector can show that an assumption of the principle direction might be incorrect.

The expected best instrumental resolutions for the detector positions as determined from simulations of the instrument are given in Fig. 6.

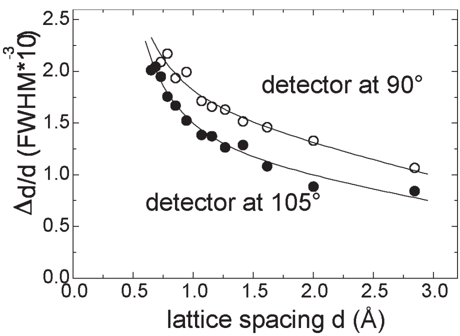

Fig. 7: *Expected best resolution of POLDI for the two detector positions.*

Conclusion

POLDI, a novel type of time-of-flight-diffractometer for strain field scanning will soon go in operation at SINQ. The main advantage of this type of instrument is that it can be optimised to high flux and high resolution, and that this optimisation can be adapted to the task of the instrument. The high intensity is achieved by using many pulses of the chopper simultaneously which can be separated by evaluation of the scattering angle-time-pattern. A best resolution of about $1.5 \cdot 10^{-3}$ is expected for the diffractometer.

References:

[1] John Scott Russel in “Report of the fourteenth meeting of the British Association for the Advancement of Science”, York, September 1844 (London 1845), pp 311-390, Plates XLVII-LVII.

[1] P. Hiismäki, *Neutron Inelastic Scattering, conf. Proc.,* p. 429, Vienna, IAEA (1972)

[2] J. K. Cockcroft and G. J. Kearley, J. Appl. Cryst. **17,** 464 (1984)

[3] U. Stuhr, Physica B **241-243,** 224 (1998)

[4] POLDI homepage: http//poldi.web.psi.ch

New SGN/SSDN members

During the course of the year 2001 we could welcome seven new members in our society, namely

- Georg Artus, Universität Zürich
- Jochen Stahn, LNS, PSI&ETHZ
- Denis Sheptyakov, LNS, PSI&ETHZ
- Stine Nyborg Klausen, Risø National Laboratory, DK
- Oksana Zaharko, LNS, PSI&ETHZ
- Christian Rüegg, LNS, PSI&ETHZ
- Fanni Juranyi, Universität des Saarlandes, DE

Presently the SGN/SSDN has 200 members.

European Funds for SINQ

Due to the still missing ratification of the bilateral agreements between the ‘EU’ and Switzerland the Swiss ‘Bundesamt für Bildung und Wissenschaft, BBW’ has agreed to fund the whole SINQ project of ‘Access to Research Infrastrucures’ for the allocated duration of 28 months by itself. The total amount of funding (€ 1.166.667,-) and the criteria for eligibility are not affected. The official start of the project now is 01/12/2001.

Next SINQ proposal deadline

The next deadline for the submission of SINQ proposals will be **May 15, 2002**

PSI mailing list

If you wish to receive a hardcopy of the PSI and/or the FUN annual reports and you did not so far please register for the PSI mailing list under the following web address:

http://www.psi.ch/news_events/news_events_info_material.shtml

Conferences 2002

date	place	conference
25.-27.1.	Heidelberg	Flexibility and Function of Proteins http://biocomp.uni-hd.de/ess-ws/
17.2.-28.3.	Grenoble	HERCULES (Research Course for Users of Neutron & Synchroton Radiation) www.polycnrs-gre.fr/hercules.html
18.-22.3.	Indianapolis	APS Conference on Condensed Matter Physics www.aps.org/meet/MAR02/abs.html
7.-11.4.	Brighton	19th General Conference of the Condensed Matter Division EPS Physics.iop.org/IOP/Confs/CMD19
9.-11.5.	Poznan	9th Int. Seminar on Neutron Scattering Investigations of Condensed Matter Nawrocik@main.amu.edu.pl
15.-17.5.	Bonn	European Neutron Scattering User Meeting
23.5.-2.6.	Erice, IT	International School of Crystallography
25.5.-1.6.	Bombannes	Scattering Methods Applied to Soft Condesed Matter www.ill.fr/Events/bombannes2002
26.-31.5.	Giens (F)	11èmes Journées de la Diffusion Neutronique Jdn11@univ-tln.fr
9.-14.6.	St. Petersburg	14th International Symposium on Boron, Borides and Related Compounds maria.korsukova@pop.ioffe.rssi.ru
1.-6.6.	Giens (F)	International Conf. on Superconductivity, GMR and Related Materials: Novel Trends a.bussmann-holder@fkf.mpg.de
10.-13.7.	Cracow	Int. Conference on Strongly Correlated Electron Systems (SCES 2002)

date	place	conference
13.-18.7.	Davis, USA	23rd Rare Earth Research Conference www.cevs.ucdavis.edu/Cofred/Public
14.-19.7.	Florence	4th Int. Conf. on ‘Science and Engineering of High-T_c Superconductivity’ www.dinamica.it/cimtec
1.-5.8.	Rigi, CH	Crystal Physics, Measuring, calculating and predicting physical properties of crystals www.kristall.ethz.ch/DGK/aks/ak5/rigi2002.html
4.-6.8.	PSI Villigen	Neutron and Synchroton X-Ray Scattering in Cond. Matter Research (IUCr-Satellite)
4.-9.8.	Houston	Applied Superconductivity Conference www.ascinc.org
6.-15.8.	Geneva	19th IUCr Congress
10.-16.8.	Zuoz, CH	PSI Summer School on Condensed Matter Research: Magnetism
11.-14.9.	Jülich/Aachen	1st Summer School on Polarized Neutron Scattering www.fz-juelich.de/iff/termine/PNCMI-2002
16.-19.9.	Jülich/Aachen	International Workshop on Polarized Neutrons for Condensed Matter Investigations www.fz-juelich.de/iff/termine/PNCMI-2002

International Conference on Neutron Scattering ICNS (09/09-13/09/2001, Munich)

A. Furrer
Laboratory for Neutron Scattering, ETHZ & PSI

Between 09/09 and 13/09/2001 about 850 participants from more than 40 countries gathered in Munich for the largest international conference on neutron scattering so far.

The scientific programme with 6 plenary and 150 contributed talks as well as 800 poster contributions covered almost all aspects of condensed matter research. The presented results impressively evidenced the broad range of applications of neutron scattering from 'hot topics' in solid state physics (e.g. high temperature superconductivity and giant magnetoresistance), chemistry (e.g. dynamics of organic molecules), biology (e.g. function of water in proteins and membranes), soft condensed matter (e.g. dynamics of polymer chains) and materials research (e.g. multilayers or nanocrystalline matter) to industrial applications like tomography and residual strain and stress analysis.

The third day of the conference was devoted to the new research reactor 'FRM-II' of the Technical University Munich in Garching. After a plenary session on neutron sources the participants got the opportunity to visit the reactor and its buildings which is almost ready to deliver neutrons. Another 'highlight' of the conference was the presentation of the prestigious 'Walter-Hälg-Prize' to Jane Brown/ILL for her life's work achievement in the field of magnetic neutron scattering.

The Swiss neutron scattering community was well represented with approximately 40 participants. Their presented results documented clearly the high scientific level of experiments performed at SINQ as well as the excellent quality of the SINQ instruments. Concerning instrumental aspects the PSI developments in the fields of neutron optics and detector electronics received great interest. The high scientific standard of the Swiss contributions was shown e.g. by the presentation of one out of five 'Young Scientist Awards' to the LNS Ph.D. student Christian Rüegg among almost 100 applicants.

A conference in Munich would not be possible without making use of the legendary 'Bavarian national drink' made from hop and malt. The participants could test several kinds during the poster session and the banquet in the traditional 'Löwenbräukeller'. This was even more appreciated since the 'Biergärten' in Munich could not be used due to the rainy weather during the days of the conference.

Fig. 1: *Ph.D. student Christian Rüegg (second from right) and his colleagues during the ceremony of the presentation of the 'Young Scientist Award'. They are flanked by the chairmen of both the conference (Winfried Petry, right) and the European Neutron Scattering Association (Bob Cywinski, left).*

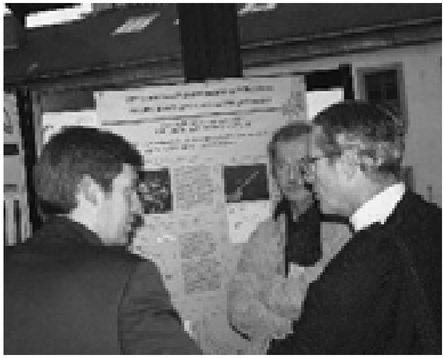

Fig. 2: *SGN/SSDN member Peter Fischer during one of the poster sessions.*

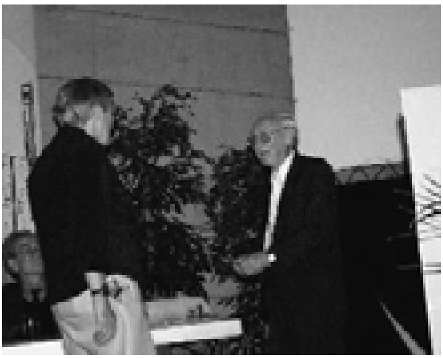

Fig. 3: *Presentation of the 'Walter-Hälg-Prize' to Jane Brown by the donor.*

Fig. 4: *Joel Mesot (PSI, second from right) and Peter Böni (TU Munich, second from left) during the visit of the instruments at the new reactor FRM-II.*

PSI Hosts First Swiss-Danish Workshop on Neutron Scattering

S. Janssen
Laboratory for Neutron Scattering, ETHZ & PSI

The cooperation between PSI and Risø National Laboratory on neutron scattering is well underway since the beginning of 2001. Since then it has undergone decisive progress mainly visible by the installation of the RITA-II triple-axis spectrometer that was completed in early summer. Two further Danish instruments namely a small angle scattering facility and another triple-axis instrument of the RITA-type will be installed during the next 12 months.

From the very beginning the cooperation was not meant to be only instrumental but also scientific. There should be a strong interaction between the two user communities where both could benefit from. A few cooperations between Swiss and Danish neutron users have already been established since several years. To strengthen those and initiate new interactions a joint 'Swiss-Danish Workshop on Neutron Scattering' was held at PSI on Nov 16/17, 2001. The workshop addressed the two topics 'Strongly Correlated Electron Systems' and 'Soft Condensed Matter', where the largest overlap from both communities is expected.

The workshop was attended by 57 participants out of which 19 came from Denmark, 32 from Switzerland and 6 from other European countries.

The program started with a welcome address from Prof. R. Eichler (PSI) and Prof. J. Kjems (Risø) on behalf of the two institutes. After that the first plenary session on 'Soft Condensed Matter' was opened with talks on 'Structure and Interaction of Block Copolymer Micelles' (J.S. Pedersen, Univ. Aarhus) and 'Strongly Interacting Colloidal Suspensions and Gels' (P. Schurtenberger, Univ. Fribourg). It was followed by a second plenary session on 'Strongly Correlated Electron Systems'. The two speakers (A. Abrahamsen, Risø and N. Cavadini, PSI) talked about 'Vortex Phases in Boron Carbide Superconductors' and 'Spin Excitations in Selected Quantum Antiferromagnets', respectively. The first day of the meeting was closed with the workshop dinner held in the PSI-restaurant 'OASE' which served a delicious menu.

On the second day the particiapnts could choose from two parallel sessions on both workshop topics. In those sessions mainly young scientists and Ph.D. students had the opportunity to present their work. The sessions showed up several highly interesting contributions. Lists with all participants, contributions and abstracts are available from the workshop-website (http://sgn.web.psi.ch/sgn/workshop.html).

Besides the scientific sessions there was enough time left for lifely and fruitful discussions. Several new contacts could be established. After the final visits of SINQ and SLS the participants left the workshop with the impression that this will not have been the last Swiss-Danish Workshop on Neutron Scattering.

Fig. 1: *The participants of the first 'Swiss-Danish Workshop on Neutron Scattering' at PSI.*

SINQ **Swiss Spallation Neutron Source** **RESEARCH PROPOSAL**	**Paul Scherrer Institute (PSI)** *SINQ* Scientific Coordination Office WHGA/147, CH-5232 Villigen PSI, Switzerland Phone: +41 56 310 2087, Fax: +41 56 310 2939 Email: SINQ@psi.ch, Web: sinq.web.psi.ch

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:

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

Anmeldeformular / Registration Form

Name / Surname ……………………………………………………………………

Vorname / First Name…………………………………………………………..……..

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Datum / Date Unterschrift / Signature

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