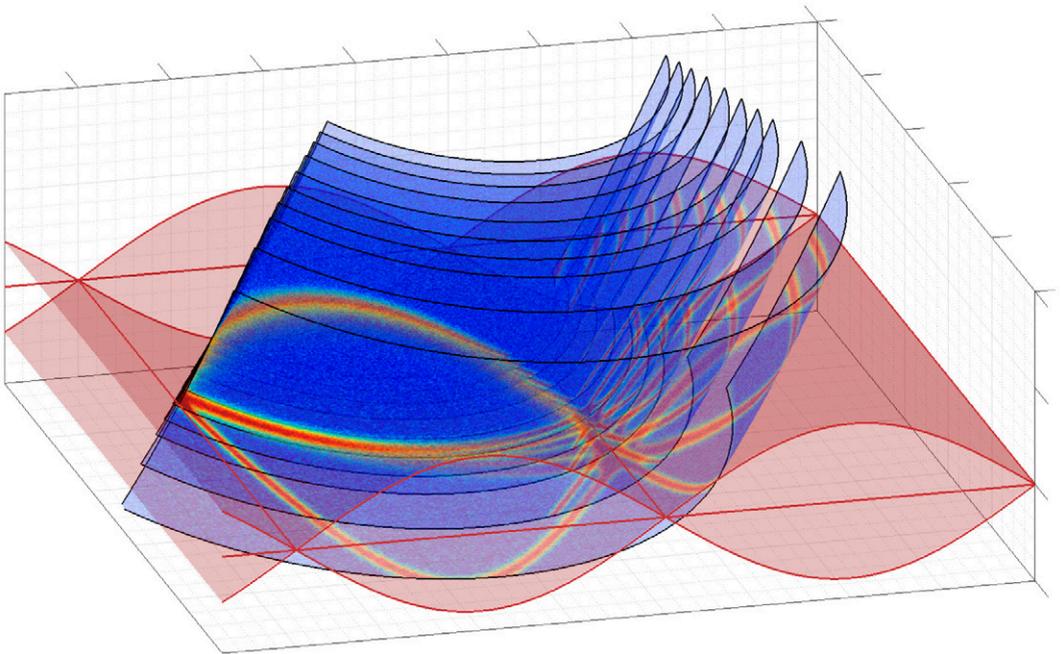


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# SWISS NEUTRON NEWS



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



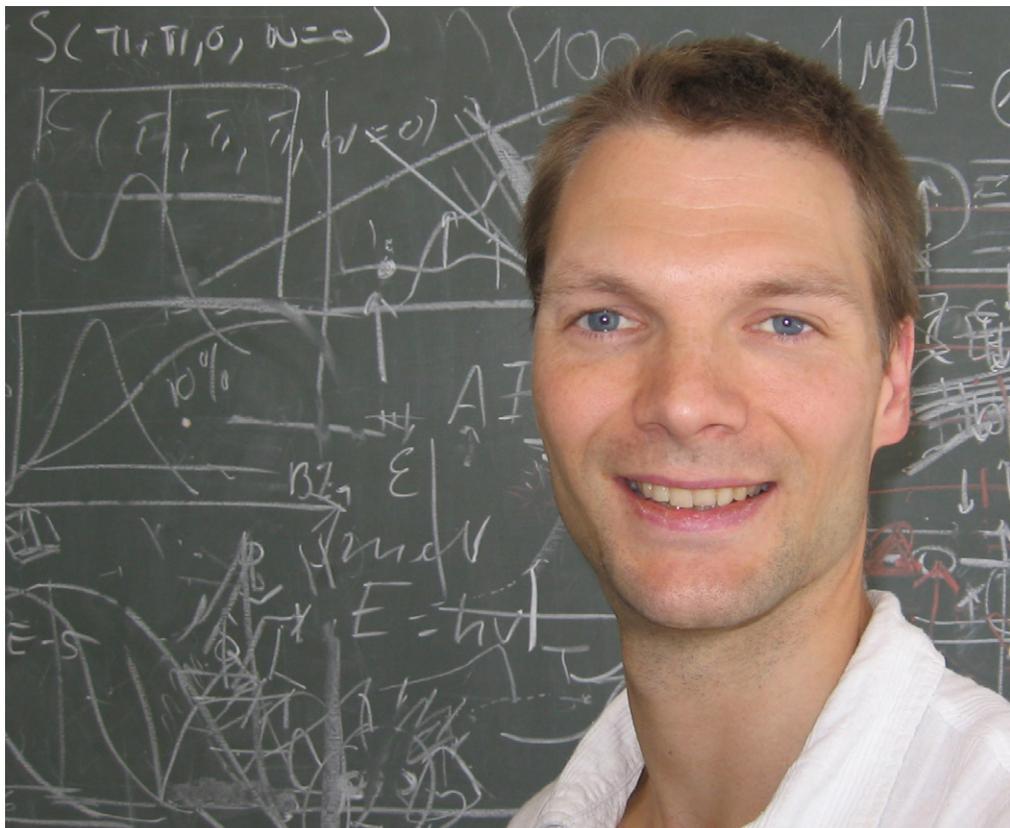
**On the cover**

Illustration of data from a single CAMEA data acquisition. See the related article "Design of the Bifrost spectrometer for ESS" by Jonas O. Birk et al.

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## The President's Page



Dear Colleagues,

In preparation for this president's word I just read what I wrote in the previous issue of Swiss Neutron News about flagship and work-horse experiments and the need to consider

the global picture when linking allocation and funding of neutron beam-time. In fact this topic remains at the top of my message board, but no point repeating it here.

Instead, let me advertise one very positive news: the acceptance of the EU project



SINE2020 "Science and Innovation with Neutrons in Europe in 2020". I congratulate both the SINE2020 and the NMI3 teams. Unlike the NMI3s, SINE2020 does not encompass EU funding of access programs, but this coming spring there is another chance at that. In this

context, let me urge each of you to explain to non-neutron scattering colleagues and policy makers the merits and needs of neutron scattering in the decades to come. To this end ENSA has compiled a short brochure "Neutrons for Science and Technology", which you can download from the ENSA web-page. The plan is to update it iteratively with new success stories, so please share with us any recent favourite examples you may have.

Or, even better, use 2016 to do some cool experiments and produce high-light examples of neutron use yourself ☺

Happy new year! May 2016 bring you excitement and surmountable challenges.

Henrik M. Ronnow

# Neutron Scattering in Switzerland in the 20th Century

**Peter Fischer and Albert Furrer**

Laboratory for Neutron Scattering

Paul Scherrer Institut, CH-5232 Villigen PSI,  
Switzerland

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## 1. Introduction

In two earlier issues of Swiss Neutron News we described the development of neutron diffractometers [1] and neutron spectrometers [2] at the Swiss neutron sources (light-water reactor Saphir 1957-1993, heavy-water reactor Diorit 1960-1977, spallation neutron source SINQ 1996-present) located at Würenlingen/Villigen from the early days up to the present. This information is complemented here by a summary of characteristic scientific and applied results which were obtained with use of the Swiss instruments for neutron scattering in the 20th century.

After the commissioning of the reactor Saphir in the year 1957, an organization called Delegation für Ausbildung und Hochschulforschung (Delegation AF) headed by Walter Hälg was installed at Würenlingen in order to educate students in the field of reactor technology as well as to initiate research with neutrons. Walter Hälg immediately recognized the potential of this new technique for materials research and started to build instruments for neutron scattering experiments. In the year 1972, the Delegation AF was transferred into the Institute for Reactor Technique (ETH Zurich) also headed by Walter Hälg. After his retirement in the year 1984, the neutron scattering activities were continued within the newly founded Laboratory for Neutron Scat-

tering (ETH Zurich) headed by Albert Furrer, which became a joint venture with the Paul Scherrer Institute (PSI) at Villigen in the year 1992. In the nineties neutron scattering studies were also carried out by members of the Abteilung Spallationsneutronenquelle at PSI.

Nearly 1200 papers were published as a result of neutron scattering experiments performed at Würenlingen/Villigen in the 20th century. This was accomplished with a relatively small number of staff members listed in Table 1. The staff members made a special effort to attract young and talented students to start their scientific careers at Würenlingen/Villigen by performing neutron scattering studies in the framework of Ph.D. theses (see Table 2). In addition, many post-doctoral students and guest scientists contributed to the scientific output. From the very beginning in the sixties, a large number of neutron scattering studies were performed in cooperation with a broad national and international user community. In this respect, the user system was introduced at the Swiss neutron sources a long time before it was copied later by most

of the neutron scattering centers around the world. The cooperations with Swiss scientists listed in Table 3 were essential to maintain a permanent home base for neutron scattering experiments in Switzerland. More specifically, the strong national user community was able to exert sufficiently strong pressure to change the plans for an early shutdown of the reactor Saphir, to establish the Swiss partnership with the Institut Laue-Langevin (ILL) at Grenoble in the year 1988 as well as to get the green light for the construction of the spallation neutron source SINQ.

In the following sections we try to focus on particular highlights resulting from neutron scattering experiments in the different decades of the 20th century. Our selection is somewhat subjective and by no means complete in terms of a professional review, but it should be regarded as being representative for the particular decade. Of course, given the names, affiliations, and thesis topics listed in Tables 1-3, more complete information can easily be obtained from the web of science.

- [1] 50 years of Swiss neutron diffraction instrumentation  
P. Fischer, J. Schefer, L. Keller, O. Zaharko, V. Pomjakushin, D. Sheptyakov, N. Aliouane, M. Frontzek, S. L. Holm, K. Lefmann, and M. Christensen, *Swiss Neutron News* No. 42, August 2013 ([http://sgn.web.psi.ch/sgn/snn/snn\\_42.pdf](http://sgn.web.psi.ch/sgn/snn/snn_42.pdf))
- [2] On the history of neutron spectrometers in Switzerland  
A. Furrer, *Swiss Neutron News* No. 43, March 2014 ([http://sgn.web.psi.ch/sgn/snn/snn\\_43.pdf](http://sgn.web.psi.ch/sgn/snn/snn_43.pdf))

**Table 1**

Staff positions (>3 years) of scientists involved in neutron scattering at Würenlingen/Villigen in the 20th century.

| Name             | Period         | Name                 | Period         |
|------------------|----------------|----------------------|----------------|
| Hälg Walter      | 1953 - 1984    | Zolliker Markus      | 1991 - 2004    |
| Schneider Toni   | 1964 - 1969    | Medarde Marisa       | 1992 - present |
| Truninger Edwin  | 1964 - 1967    | Mesot Joël           | 1992 - 2008    |
| Fischer Peter    | 1966 - 2002    | Allenspach Peter     | 1993 - 2004    |
| Bührer Willi     | 1969 - 1997    | Clemens Daniel       | 1994 - 2002    |
| Furrer Albert    | 1970 - 2004    | Janssen Stefan       | 1995 - 2004    |
| Benes Josef      | 1970 - 1982    | Keller Lukas         | 1996 - present |
| Millhouse Arthur | 1971 - 1975    | Kohlbrecher Joachim  | 1996 - present |
| Tichy Karel      | 1972 - 1984    | Stuhr Uwe            | 1996 - present |
| Anderson Ian     | 1986 - 1991    | Roessli Bertrand     | 1997 - present |
| Schefer Jürg     | 1987 - present | Altorfer Felix       | 1998 - 2002    |
| Böni Peter       | 1988 - 2000    | Zaharko Oksana       | 1998 - present |
| Wagner Werner    | 1990 - 2014    | Pomjakushin Vladimir | 1999 - present |

**Table 2**

Ph.D. theses in neutron scattering carried out at Würenlingen/Villigen in the 20th century.

| Name                | Period    | Topic  |
|---------------------|-----------|--|
| Fischer Peter       | 1961-1966 | Neutron diffraction studies of $\text{MgAl}_2\text{O}_4$ and $\text{ZnAl}_2\text{O}_4$ |
| Stoll Erich         | 1963-1968 | Lattice dynamics and electronic properties of Mg                                       |
| Bührer Willi        | 1964-1969 | Lattice dynamics of copper   |
| Furrer Albert       | 1965-1970 | Lattice dynamics of lead at different temperatures                                     |
| Waeber Waldemar     | 1966-1969 | Lattice vibrations of gallium  |
| Lutz Ulrich         | 1966-1970 | Lattice dynamics of anthracene   |
| Von Wartburg Werner | 1969-1973 | Magnetic structure of $\text{Ni}_2\text{B}_7\text{O}_{13}$                             |
| Heer Heinz          | 1970-1978 | Neutron spectroscopic studies of the Ce monopnictides                                  |
| Meier Guido         | 1972-1977 | Magnetic ordering in the Ce monopnictides  |
| Tellenbach Ulrich   | 1974-1977 | Spin waves in $\text{CsNiCl}_3$ and $\text{CsCoCl}_3$                                  |

| Name                  | Period    | Topic   |
|-----------------------|-----------|---|
| Schefer Jürg          | 1979-1983 | Structural studies of metal hydrides  |
| Hälg Beat             | 1980-1984 | Spin dynamics of Ce and U mononpnictides  |
| Falk Urs              | 1981-1984 | Magnetic exchange interactions in $\text{CsMn}_x\text{Mg}_{1-x}\text{Br}_3$   |
| Stöckli Armin         | 1983-1987 | Dynamics of hydrogen bonds in carboxylic acids  |
| Schmid Beat           | 1984-1988 | Neutron studies of Pr and U trihalogenides and $\text{Tb}_2\text{Cl}_3$   |
| Dönni Andreas         | 1987-1991 | Neutron studies of $\text{CeX}$ ( $\text{X}=\text{S},\text{Se}$ ) and $\text{YbX}$ ( $\text{X}=\text{N},\text{P},\text{As},\text{Sb}$ ) |
| Elsenhans Olivier     | 1987-1991 | Crystal-field interaction in $\text{RPd}_3$ ( $\text{R}=\text{Dy},\text{Er},\text{Tm},\text{Yb}$ )                                      |
| Zolliker Markus       | 1987-1991 | Neutron studies of the shape-memory compounds $\text{CuZnAl}$   |
| Allenspach Peter      | 1988-1991 | Neutron spectroscopic studies of high- $T_c$ superconductors  |
| Rüdlinger Martin      | 1988-1992 | Light induced structural changes in Na nitrosylprussiate  |
| Meso Joël             | 1989-1992 | Crystal-field interaction in Er based high- $T_c$ compounds   |
| Staub Urs             | 1989-1993 | Crystal-field and exchange effects in high- $T_c$ compounds   |
| Altorfer Felix        | 1990-1994 | Neutron studies of ionic conductors   |
| Guillaume Michel      | 1991-1994 | Neutron studies of high- $T_c$ superconductors  |
| Keller Lukas          | 1991-1994 | Neutron studies of lanthanide and actinide compounds  |
| Roessli Bertrand      | 1991-1994 | Neutron studies of $\text{HoBa}_2\text{Cu}_4\text{O}_8$ , $\text{Bi}_2\text{CuO}_4$ , and $\text{CeGeO}_3$                              |
| Fauth François        | 1992-1996 | Neutron studies of oriented $\text{HoBa}_2\text{Cu}_3\text{O}_x$ and $\text{ErBa}_2\text{Cu}_3\text{O}_7$                               |
| Marti Willi           | 1992-1995 | Neutron studies of $\text{RGaO}_3$ ( $\text{R}=\text{La},\text{Pr},\text{Nd}$ ) and $\text{NdBa}_2\text{Cu}_3\text{O}_7$                |
| Rosenkranz Stefan     | 1992-1996 | Neutron studies of $\text{RNiO}_3$ ( $\text{R}=\text{rare earth}$ )   |
| Henggeler Wolfgang    | 1993-1996 | Neutron studies of magnetic correlations in cuprates  |
| Böttger Grit          | 1994-1998 | Neutron studies of rare-earth based high- $T_c$ compounds   |
| Löffler Jörg          | 1994-1997 | Properties of nanostructured Fe, Co and Ni  |
| Gasser Urs            | 1995-1999 | Magnetic properties of $\text{RNi}_2\text{B}_2\text{C}$ ( $\text{R}=\text{rare earth}$ )  |
| Gutmann Matthias      | 1995-1999 | Local inhomogeneities of high- $T_c$ superconductors  |
| Tixier Sebastien      | 1997-2000 | Structural characterization of metallic multilayers   |
| Semadeni Fabrizio     | 1997-2000 | Spin fluctuations in magnetically ordered systems   |
| Cavadini Nordal       | 1998-2001 | Magnetic correlations in quantum spin systems   |
| Herrmannsdörfer Thilo | 1998-2002 | Neutron studies of strongly correlated electron systems   |
| Rubio Daniel          | 1998-2002 | Pseudogap and isotope effects in high- $T_c$ compounds  |
| Böhm Martin           | 1999-2002 | Magnetic neutron scattering studies of $\text{CuB}_2\text{O}_4$   |
| Schaniel Dominik      | 1999-2002 | Structure of high knowledge content materials   |
| Strässle Thierry      | 1999-2002 | Cooling by the barocaloric effect in rare-earth compounds   |

**Table 3**

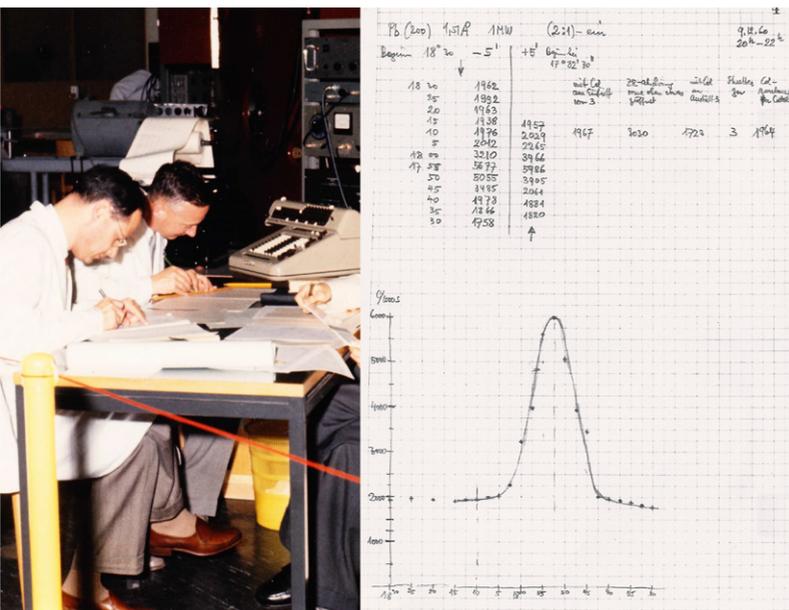
Cooperations in neutron scattering established with Swiss research institutions in the 20th century.

| <b>Organization</b> | <b>Institute</b>          | <b>Professors and Senior Scientists</b>   |
|---------------------|---------------------------|---|
| ABB Dättwil         | Research Center           | P. Brüesch, T. W. Duerig, R. S. Perkins   |
| EPF Lausanne        | Applied Physics           | F. Lévy   |
| EPF Lausanne        | Micro- & Optoelectronics  | H. J. Scheel  |
| EPF Lausanne        | Physics of Complex Matter | R. Gotthardt  |
| ETH Zurich          | Applied Physics           | G. Kostorz, B. Schönfeld  |
| ETH Zürich          | Cell Biology              | K. Mühlethaler  |
| ETH Zurich          | Crystallography           | Ch. Baerlocher, K. Girgis, F. Laves, A. Niggli,<br>P. Schobinger-Papamantellos, D. Schwarzenbach  |
| ETH Zurich          | Physical Chemistry        | R. R. Ernst, B. H. Meier  |
| ETH Zurich          | Solid State Physics       | H. Arend, G. Busch, F. Hulliger, E. Kaldis,<br>W. Känzig, K. Mattenberger, J. Karpinski,<br>H. R. Ott, L. Schlapbach, P. Wachter, O. Vogt |
| IBM Zurich          | Research Center           | B. Lüthi, K. A. Müller, A. Segmüller  |
| Univ. Basel         | Physics                   | H. J. Güntherodt, H. Rudin  |
| Univ. Bern          | Crystallography           | H. B. Bürgi   |
| Univ. Bern          | Inorganic Chemistry       | S. Decurtins, H. Gamsjäger, H. U. Güdel,<br>K. W. Krämer, A. Ludi   |
| Univ. Fribourg      | Physics                   | L. Schlapbach, A. Züttel  |
| Univ. Geneva        | Applied Chemistry         | F. Kubel, H. Schmid, P. Tissot  |
| Univ. Geneva        | Crystallography           | R. Cerny, K. Yvon   |
| Univ. Geneva        | Physical Chemistry        | H. Bill   |
| Univ. Geneva        | Solid State Physics       | R. Flükiger, A. Junod, H. G. Purwins, E. Walker   |
| Univ. Lausanne      | Crystallography           | D. Schwarzenbach  |
| Univ. Zurich        | Inorganic Chemistry       | J. H. Ammeter   |
| Univ. Zurich        | Physics                   | K. A. Müller, F. Waldner  |

## 2. Neutron scattering in the sixties

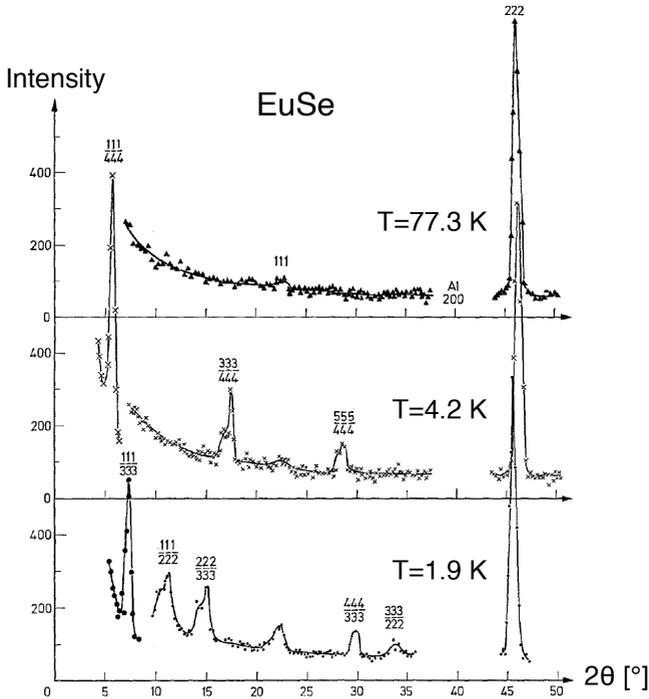
A prototype two-axis neutron diffractometer was ready for experiments in the year 1960. Fig. 1 is a historical document, displaying the very first measurement on a lead crystal performed by Walter Halg. At that time the experimental results had to be plotted manually, and calculations had to be done by slide rules (pocket calculators and PC's did not exist). Since auxiliary equipments such as cryostats, furnaces and magnets were initially lacking, the diffraction experiments mainly concentrated on room-temperature investigations to **distinguish neighboring elements or ions of the periodic table** (e.g.  $Mg^{2+}$  and  $Al^{3+}$  with equal number of ten electrons) [3] as well as to **locate light atoms** (e.g. hydrogen) in the

**presence of heavy atoms** [4], thereby demonstrating two outstanding properties of neutrons in contrast to x-rays. In order to demonstrate another important property of the neutron, namely its magnetic moment being an excellent probe to study magnetic phenomena, cooling devices were required. As a first step a liquid-nitrogen cryostat with styrofoam shielding was produced internally by the workshop group. Later a commercial liquid-helium cryostat was purchased, but its operation turned out to be rather expensive, since there was no He gas recovery system. Moreover, liquid helium had to be bought and imported from abroad, often with considerable losses during the transport. Nevertheless, clear evidence for **magnetic phase transitions** could be provided for several rare-earth compounds



**Figure 1**

Walter Halg (right) plots the data of the first neutron diffraction experiment performed for a single crystal of lead at the reactor Saphir (1 MW) in the year 1960 [1.5 Angstrom neutron (200) intensity versus Bragg angle  $\theta$  in the  $\theta$ - $2\theta$  mode].



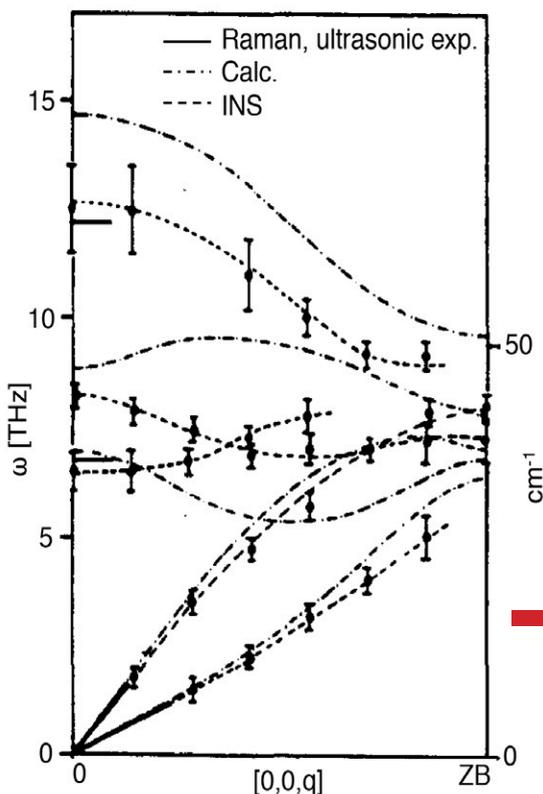
**Figure 2**

Neutron single crystal [1,1,1] scans of EuSe as a function of temperature (neutron wavelength  $\lambda=1.39 \text{ \AA}$ ). At  $T=77.3 \text{ K}$  only nuclear Bragg peaks with indices (h,h,h) are observed. At  $T=4.2 \text{ K}$  EuSe is antiferromagnetically ordered according to a (++-)-configuration and propagation vector  $\mathbf{k}=[1/4,1/4,1/4]$ . At  $T=1.9 \text{ K}$  partial ferromagnetism ( $\mathbf{k}=0$ ) is observed in the intensity increase of the nuclear Bragg peak (1,1,1), whereas the antiferromagnetic moment components are associated with the  $\mathbf{k}$  vectors  $[1/3,1/3,1/3]$  and  $[1/2,1/2,1/2]$  (after Ref. 5).

[5] as illustrated for a single crystal of EuSe (with neutron absorbing Eu) in Fig. 2.

Neutron spectroscopic experiments were initially carried out with use of a rotating-crystal time-of-flight spectrometer, later complemented by a triple-axis spectrometer. These instruments allowed to demonstrate another unique property of neutrons, namely to meas-

ure excitations at any wavevector in the Brillouin zone, in contrast to optical spectroscopies being confined to the zone center. The aim of the first experiment was to establish the **phonon dispersion** in a single crystal of copper [6]. In later experiments the phonon dispersion in single crystals of gallium and lead were studied, and finally the mapping of



the phonon dispersion curves in a single crystal of deuterated anthracene could be successfully accomplished as shown in Fig. 3 [7]. The latter study was a remarkable achievement, since at that time only little work on the phonon dispersion in organic molecular compounds was available.

**Figure 3**

Dispersion curves of deuterated anthracene. Comparison of calculated and measured data (after Ref. 7).

- [3] Redetermination of the cation distribution of spinel ( $\text{MgAl}_2\text{O}_4$ ) by means of neutron diffraction  
E. Stoll, P. Fischer, W. Hälg, and G. Maier, *J. de Physique* **25**, 447 (1964)
- [4] Neutron diffraction study of  $\text{D}_3\text{Co}(\text{CN})_6$   
H. U. Güdel, A. Ludi, P. Fischer, and W. Hälg, *J. Chem. Phys.* **53**, 1917 (1970)
- [5] Neutron diffraction evidence for magnetic phase transition in europium selenide  
P. Fischer, W. Hälg, W. von Wartburg, P. Schwob, and O. Vogt, *Phys. kondens. Materie* **9**, 249 (1969)
- [6] Phonon dispersion in copper  
W. Bühner, T. Schneider, and W. Gläser, *Solid State Commun.* **4**, 443 (1966)
- [7] Lattice dynamics of deuterated anthracene  
U. Lutz and W. Hälg, *Solid State Commun.* **8**, 165 (1970)

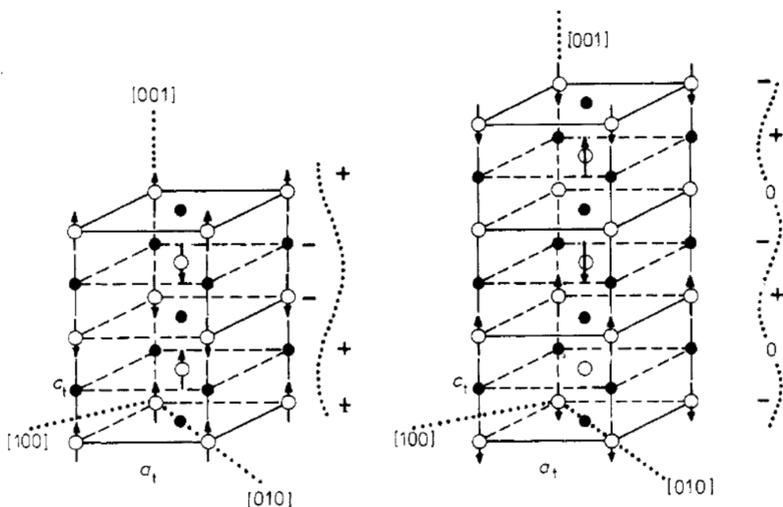
### 3. Neutron scattering in the seventies

In this decade, the instruments for neutron scattering (two diffractometers and two triple-axis spectrometers) were continuously upgraded, and the sample environment included state-of-the-art cryostats, furnaces, and magnets, allowing experiments at the forefront of science to meet the requirements of the steadily growing user community.

The neutron diffraction experiments largely concentrated on the characterization of **magnetic ordering phenomena**. Among the myriads of samples studied, we mention as an example the compound CeSb which exhibits

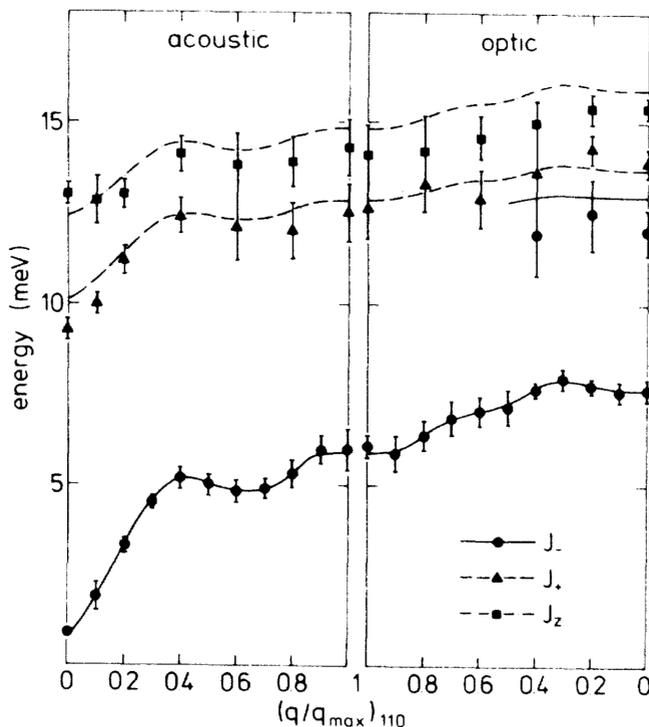
a remarkably complex magnetic phase diagram with six partially disordered magnetic phases below  $T_N=16$  K [8] as illustrated for the phases I and VI in Fig. 4. The magnetic moments are oriented along the directions  $\langle 1,0,0 \rangle$ , although the crystal-field interaction favors  $\langle 1,1,1 \rangle$  as easy directions. This is due to strongly anisotropic exchange interactions which were later established by neutron spectroscopy (see section 4 and Ref. 17).

Consecutively, neutron spectroscopic experiments were carried to determine the **crystal-field interaction** in these compounds, from which the magnetic properties could be quantitatively reproduced in the mean-field approx-



**Figure 4**

Basic modulated antiferromagnetic structures of CeSb corresponding to Z domains. Left: Phase VI ( $\mathbf{k} = [0, 0, 1/2]$ ,  $T \leq 8.9$  K). Right: Phase I ( $\mathbf{k} = [0, 0, 2/3]$ ,  $T = 16.0$  K). The tetragonal magnetic unit cells are shown. Open and filled circles represent Ce and Sb atoms, respectively. Note the decreasing order from 100% to 67% in the magnetic planes with increasing temperature (after Ref. 8).



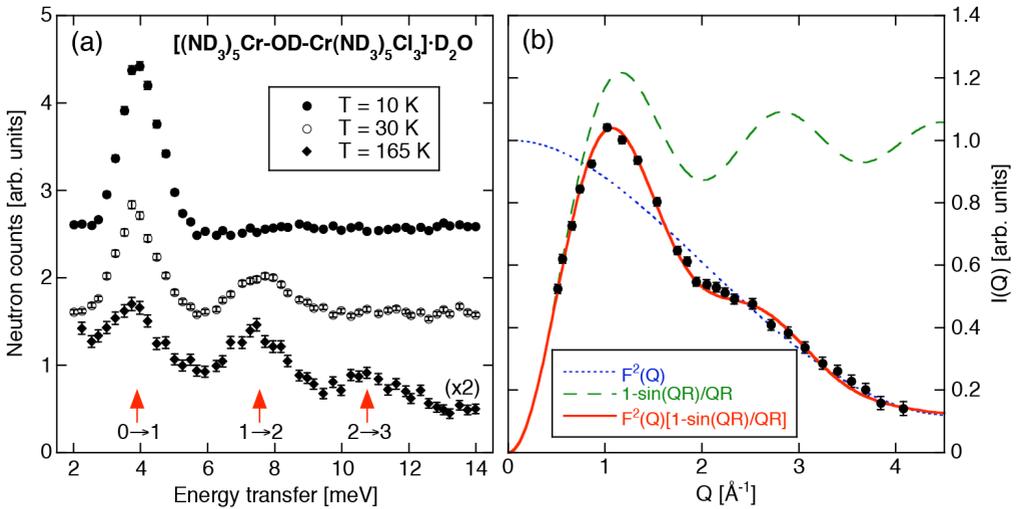
**Figure 5**

Dispersion of magnetic excitations of  $\text{NdAl}_2$  at  $T = 4.2$  K for wavevectors along the direction  $\langle 1,1,0 \rangle$ . The lines represent the best fit to a pseudoboson model that includes all ten levels of the  $\text{Nd}^{3+}$  ground-state multiplet (after Ref. 9).

imation. When single crystals were available, the dispersion of the **magnetic excitations** could be mapped, yielding additional information on the exchange interaction as exemplified for the compound  $\text{NdAl}_2$  in Fig. 5 [9].

The Middle East conflict due to the Suez crisis resulted in a worldwide shortage of oil, so that large efforts were undertaken to search for alternative energies. Hydrogen was identified as such a substituent, and neutron

scattering was the ideal tool to characterize the proposed **hydrogen storage systems**. Early neutron diffraction experiments were carried out for the most promising candidates  $\text{FeTiD}_x$  and  $\text{LaNi}_5\text{D}_x$  [10] to determine the deuterium positions as a function of deuterium pressure. This information turned out to be useful to reconstruct the diffusion paths of the D atoms.



**Figure 6**

(a) Energy spectra of neutrons scattered from  $[(\text{ND}_3)_5\text{CrODCr}(\text{ND}_3)_5]\cdot\text{D}_2\text{O}$ . (b)  $Q$  dependence of the intensity of the  $|0\rangle \rightarrow |1\rangle$  transition at  $T = 4.2\text{ K}$ , exhibiting a sinusoidal modulation characteristic of the scattering from magnetic clusters (after Ref. 12).

Other efforts towards technological applications were undertaken in the field of **super-ionic conductivity**. The phonon dispersion of several silver halides provided essential information on the conductive behavior [11]. In particular, a very-low-lying dispersionless transverse optic phonon mode as well as strong anharmonic effects were observed, which can be attributed to the movement of the Ag ions.

Neutron spectroscopic experiments were started to study the excitations associated with **magnetic clusters** embedded in molecular complexes, which was a great challenge due to the small number of atoms taking part of the magnetic scattering process. Nevertheless, the first inelastic neutron scattering

experiment was successfully performed for deuterated  $[(\text{ND}_3)_5\text{CrODCr}(\text{ND}_3)_5]\cdot\text{D}_2\text{O}$  [12], in which the weight of the dimeric Cr clusters amounts to only 4 at%. As shown in Fig. 6, three well resolved transitions showed up in the experiments, so that the ground-state exchange splitting of the Cr dimer could be unambiguously determined. The scattering law for magnetic clusters developed in the course of this experiment laid the basis for the many neutron spectroscopic studies of molecular magnets which have been carried out up to the present.

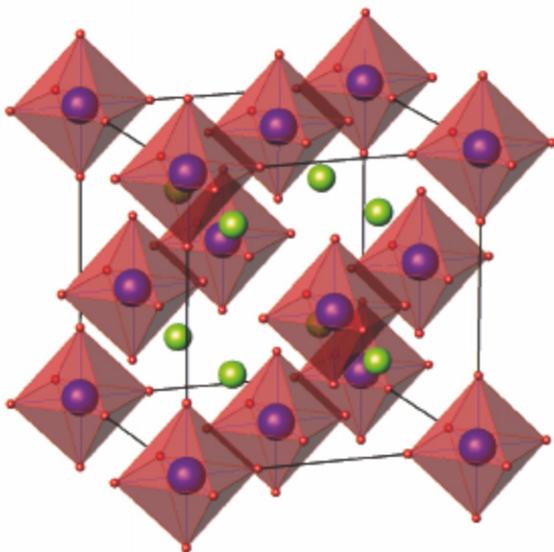
- [8] Magnetic phase transitions of CeSb. I. Zero applied magnetic field  
P. Fischer, B. Lebech, G. Meier, B. D. Rainford, and O. Vogt, *J. Phys. C* **11**, 345 (1978)
- [9] Magnetic excitations in NdAl<sub>2</sub>  
A. Furrer and H. G. Purwins, *Phys. Rev. B* **16**, 2131 (1977)
- [10] Neutron scattering investigations of the LaNi<sub>5</sub> hydrogen storage system  
P. Fischer, A. Furrer, G. Busch, and L. Schlapbach, *Helv. Phys. Acta* **50**, 481 (1977)
- [11] Lattice dynamics of silver iodide by neutron scattering  
W. Bührer, R. M. Nicklow, and P. Brüesch, *Phys. Rev. B* **17**, 3362 (1978)
- [12] Interference effects in neutron scattering from magnetic clusters  
A. Furrer and H. U. Güdel, *Phys. Rev. Lett.* **39**, 657 (1977)

#### 4. Neutron scattering in the eighties

The experimental work profitted from the availability of a dilution refrigerator to reach temperatures down to 7 mK as well as of new devices achieving uniaxial and hydrostatic pressures up to 10 GPa. On the instrumental side, the single detector of the powder diffractometer was replaced by a BF<sub>3</sub> based multidetector bank covering an angular range of 80°, and the insertion of a radial oscillating

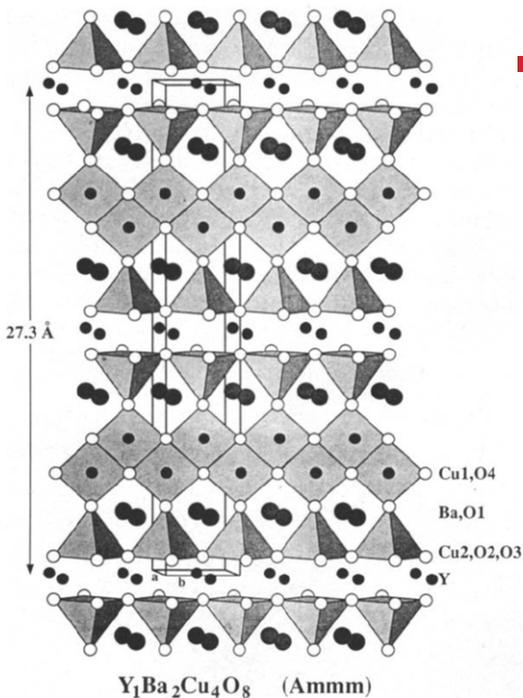
collimator was essential to remove disturbing Bragg peaks originating from the sample surroundings. The triple-axis spectrometers were equipped with large focusing monochromator and analyzer systems. All these measures resulted in intensity gain factors up to two orders of magnitude which permitted new types of experiments.

The research on many topics investigated in the seventies was continued. The structures of **novel metal hydrides** were determined as exemplified in Fig. 7 for Mg<sub>2</sub>FeH<sub>6</sub> with a remarkably high hydrogen density [13]. The study of both **magnetic ordering phenomena and magnetic excitation spectra** was extended to include more complicated ternary materials. In particular, compounds of com-



**Figure 7**

Unit cell of Mg<sub>2</sub>FeD<sub>6</sub> with Mg<sup>2+</sup> ions shown as green spheres and with the characteristic red D<sub>6</sub> octahedra around central violet Fe<sup>2+</sup> (after Ref. 13).



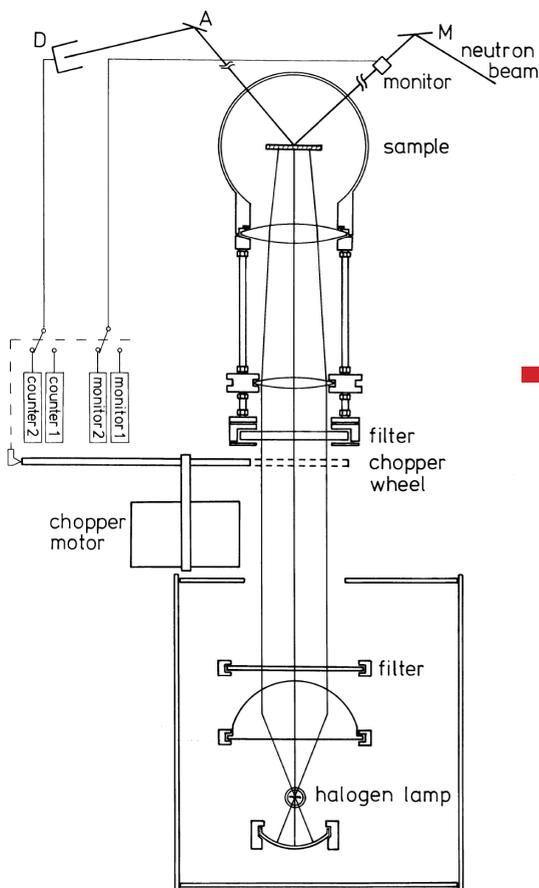
**Figure 8**

Crystal structure of the 80K superconductor  $\text{YBa}_2\text{Cu}_4\text{O}_8$  characterized by double  $\text{CuO}$  chains (after Ref. 18).

position  $\text{Cs}_3\text{A}_2\text{X}_9$  (A=transition metal or rare-earth ion, X=halogen ion) with antiferromagnetically coupled A dimers were intensively investigated due to their interest in fundamental and applied research as novel singlet-triplet systems and new candidates for highly efficient upconversion lasers, respectively. Neutron diffraction experiments gave evidence for spontaneous magnetic order induced by an intratriplet mode in  $\text{Cs}_3\text{Cr}_2\text{I}_9$  [14]. On the neutron spectroscopic side, the improved instrumental conditions allowed to observe subtle details of the magnetic excitation spectra, allowing an analysis beyond the conventional Heisenberg model in terms of higher-order and anisotropic exchange interactions [15-17].

However, the highlight of the eighties was the discovery of **high-temperature superconductivity** in doped  $\text{La}_2\text{CuO}_4$  by K. A. Müller and G. Bednorz. This set off enormous worldwide efforts to search for other superconducting oxides. Different copper-oxide superconductors of type  $\text{R}_2\text{CuO}_{4-x}$ ,  $\text{RBa}_2\text{Cu}_3\text{O}_{7-x}$ ,  $\text{RBa}_2\text{Cu}_4\text{O}_{8+x}$ , and  $\text{R}_2\text{Ba}_4\text{Cu}_7\text{O}_{15}$  (R=yttrium or rare-earth) were investigated by neutron diffraction to understand the structural and magnetic properties as a function of doping and pressure. Fig. 8 illustrates the characteristic double  $\text{CuO}$  chains of  $\text{YBa}_2\text{Cu}_4\text{O}_8$  with  $T_c=80\text{K}$  [18]. It has been realized that the superconducting transition temperature is essentially unchanged upon replacing the Y and La ions by magnetic rare-earth ions, thus neutron spectroscopic experiments to determine the magnetic ground state through the crystal-field interaction turned out to be most useful. However, an unambiguous parametrization of the crystal-field interaction (nine independent parameters are required for orthorhombic symmetry) was not a trivial task, but could successfully be achieved for the first time for the compound  $\text{HoBa}_2\text{Cu}_3\text{O}_{7-x}$  [19].

The structure and the **dynamics of protons in hydrogen bridges** was studied in a series



**Figure 9**

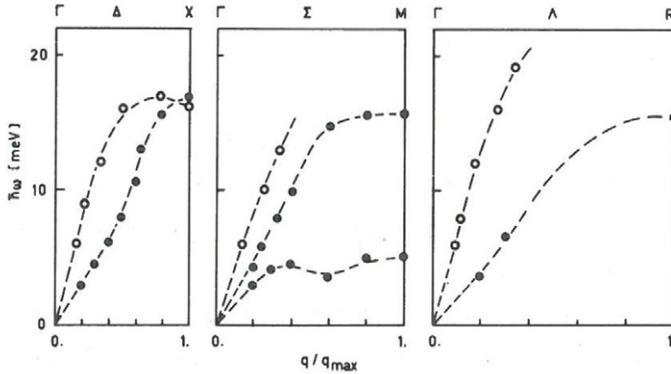
Conceptual design of the instrumental device developed for simultaneous light irradiation and neutron scattering at low temperatures. The light beam is periodically interrupted by a rotating chopper wheel with regularly arranged openings. The neutron count rates are separately stored for the "light" and "dark" experiments by the counters 1 and 2, respectively. The pulsed beam technique is essential to avoid sample heating upon illumination by light (after Ref. 21).

of dimeric carboxylic acids which are frequently used in the production of polymers, pharmaceuticals, solvents, and food additives. It has been suggested that the double proton exchange occurs through a torsional motion of the entire COOH group, but the results obtained by quasielastic neutron scattering unambiguously rejected this view in favor of a translational motion [20].

Inelastic neutron scattering experiments were started to investigate **photoeffects on the dynamical properties** of chlorophyll mol-

ecules embedded in membranes. A special device was developed to allow the simultaneous irradiation of the sample by neutrons and light at low temperatures as shown in Fig. 9 [21]. The illumination by light results in a partial freezing of rotational modes which may be attributed to a possible coupling with particular mechanisms of the photosynthetic process.

The compound NiTi exhibits a thermoelastic martensitic phase transformation at  $T_m=278$  K. After a special thermomechanical



**Figure 10**  
Phonon dispersion curves  
observed for the  
shape-memory compound  
NiTi at  $T=293$  K (after Ref.  
22).

treatment the transition is associated with a reversible shape change when the temperature is cycled around  $T_m$ . The **shape-memory mechanism** is reflected in unusual features of the phonon dispersion curves as shown in

Fig. 10 [22]. More specifically, the transverse acoustic phonon modes exhibit a convex behavior and a dip along the  $\langle 1,1,0 \rangle$  direction which are considered as precursor effects of the martensitic phase transition.

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K. Yvon and P. Fischer, Hydrogen in intermetallic compounds I, *Topics in Applied Physics* 63  
(Ed. L. Schlapbach, Springer-Verlag, Berlin 1988) p. 87
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B. H. Meier, R. Meyer, R. R. Ernst, A. Stöckli, A. Furrer, W. Hälgl, and I. Anderson, *Chem. Phys. Lett.* 108, 522 (1984)
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## 5. Neutron scattering in the nineties

At the end of 1993 the reactor Saphir was finally shut down, but the regular operation of the spallation neutron source *SINQ* started only in mid-1998. In order to avoid the threatening neutron gap, a Swiss neutron base was established at the ILL Grenoble from 1995-1998 in the framework of a "collaborating research group", giving exclusive access to the three-axis spectrometer IN3 (100%) and the powder diffractometer D1A (50%). The imposed limited access to Swiss instruments

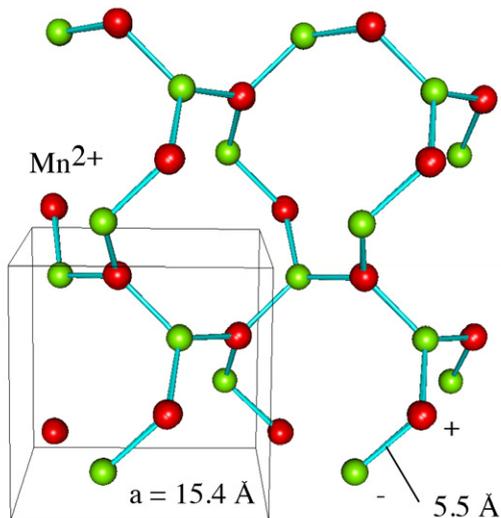
in the mid-nineties allowed the staff members (see Fig. 11) to engage themselves in the organization of the first European Conference on Neutron Scattering in Interlaken (ECNS 1996), which featured a record attendance of more than 700 participants.

Many fascinating results were obtained by both neutron diffraction and neutron spectroscopic experiments on multiferroic systems (e.g.  $\text{KNiPO}_4$ ), **heavy-fermion superconductors** (such as the highly cited compound  $\text{UM}_2\text{Al}_3$  with  $M=\text{Pd}, \text{Ni}$  [23]), Kondo compounds (e.g.  $\text{YbCu}_4M$  with  $M=\text{Au}, \text{Pd}$ ), and "free-electron"



**Figure 11**

The organizing committee of the 1st European Conference of Neutron Scattering (ECNS 1996) in Interlaken. Front row (from left to right): J. Duppich, R. Bercher, A. Furrer, J. Granella, W. Fischer. Back row: J. Mesot, J. Schefer, P. Fischer, H. Heer, P. Allenspach, W. Bührer, P. Böni, W. Wagner, G. Bauer.



**Figure 12**

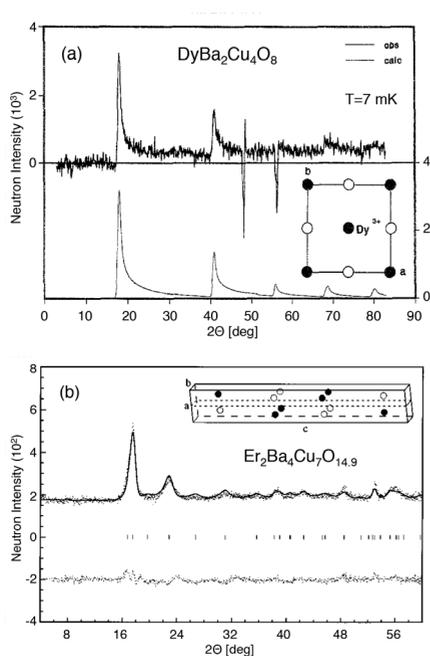
Antiferromagnetic  $\text{Mn}^{2+}$  ordering (shown by red and green spheres indicating antiparallel moment orientation) in supramolecular  $\text{Mn}_2\text{FeC}_{36}\text{D}_{24}\text{N}_6\text{O}_{12}$  below  $T_N=13 \text{ K}$ .  $\mu_{\text{Mn}}=4.6(1) \mu_B$  at  $T=1.8 \text{ K}$  (after Ref. 24).

rare-earth halides (e.g.  $\text{R}_2\text{X}_5$  with  $\text{R}=\text{Ce}, \text{Pr}$  and  $\text{X}=\text{Br}, \text{I}$ ). Outstanding concerning novelty was the study of three-dimensional chiral, oxalate-bridged **supramolecules containing magnetic ions** such as  $\text{Fe}^{2+}$  and  $\text{Mn}^{2+}$ . This is exemplified in Fig. 12 for  $\text{Mn}_2\text{FeC}_{36}\text{D}_{24}\text{N}_6\text{O}_{12}$  in which three-dimensional antiferromagnetic  $\text{Mn}^{2+}$  ordering was found below  $T_N=13 \text{ K}$ , whereas iron does not order magnetically [24].

The research on **high-temperature superconductors** was continued. A systematic neutron diffraction study of the compounds  $\text{RBa}_2\text{Cu}_3\text{O}_x$  ( $\text{R}=\text{yttrium}$  and rare earths,  $x=6$  and  $7$ ) nicely showed how the apex oxygen position monitors changes of the charge distribution in the copper-oxide planes [25]. Efforts were undertaken to study the coexistence of superconductivity and magnetic ordering in the mK range due to the rare-earth ions [26] as shown in Fig. 13 for both the two-dimensional Dy ordering in  $\text{DyBa}_2\text{Cu}_4\text{O}_8$  and the three-dimensional Er ordering in  $\text{Er}_2\text{Ba}_4\text{Cu}_7\text{O}_{14.9}$ . Neutron spectroscopic studies of the crystal-field spectra gave evidence for

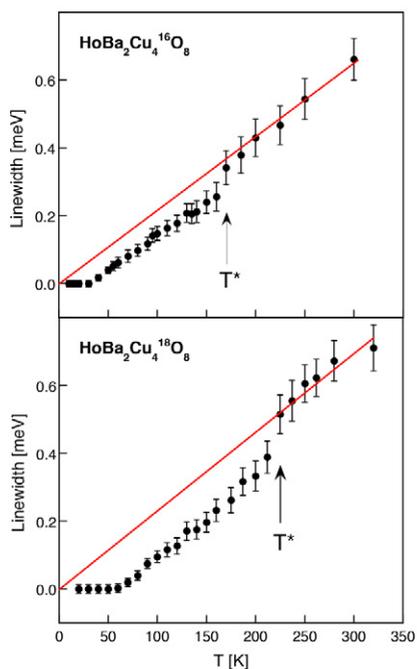
a superposition of local regions of semiconducting and metallic character [27], thereby confirming the percolative nature of high-temperature superconductivity. In addition, by studying the relaxation rate of crystal-field excitations large oxygen and copper isotope effects on the pseudogap were observed as shown in Fig. 14 [28], giving support for the importance of electron-phonon induced effects in any model for high-temperature superconductivity. The International Science Index (ISI) identified Ref. 28 for the whole field of physics as a so-called Fast Breaking Paper which corresponds to the top 1% of highly cited papers having the largest bimonthly increase of citations in 22 broad fields of science.

As a consequence of the hype with high-temperature superconductors, the neutron scattering studies of the cuprates were extended to **other perovskites** such as rare-earth based manganates, nickelates, and gallates, which exhibit interesting physical properties as a function of temperature, pres-



**Figure 13**

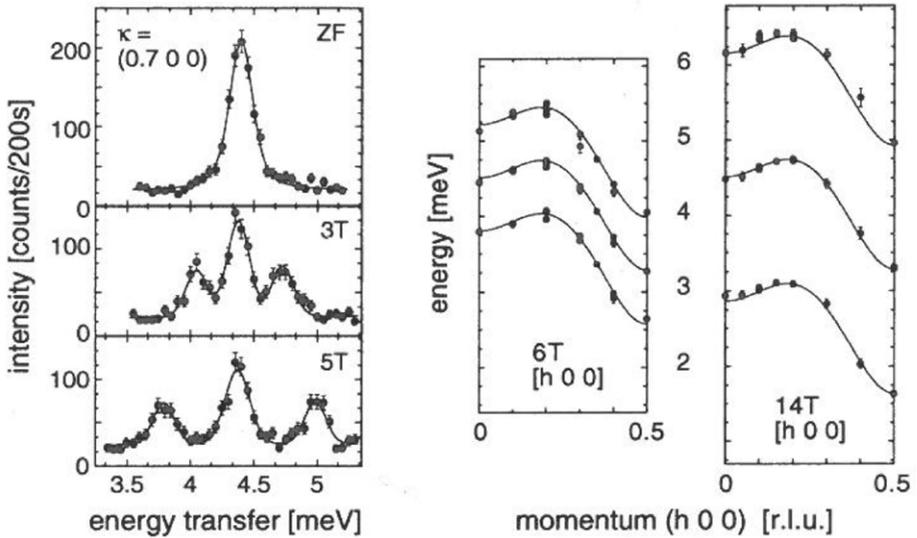
(a) Two-dimensional antiferromagnetic Dy<sup>3+</sup> ordering in DyBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> at 7 mK and corresponding magnetic difference neutron diffraction pattern (7 mK - 1.2 K) from DMC. The observed points are corrected for paramagnetic diffuse scattering. Filled and open circles indicate antiparallel alignment of the magnetic moments perpendicular to the (a,b) plane. (b) Three-dimensional magnetic Er<sup>3+</sup> ordering in superconducting Er<sub>2</sub>Ba<sub>4</sub>Cu<sub>7</sub>O<sub>14,9</sub>, corresponding to  $k=[0,1/2,1/2]$  and associated magnetic difference neutron diffraction pattern (25 mK - 3 K), measured on D1A at ILL. Black and white spheres indicate antiferromagnetic ordering with the magnetic moments oriented parallel to the b-axis;  $T_c=89 \text{ K}$  and  $T_N=0.54 \text{ K}$  (after Ref. 26).



**Figure 14**

Temperature dependence of the intrinsic linewidth of the lowest ground-state crystal-field transition in  $\text{HoBa}_2\text{Cu}_4^{16}\text{O}_8$  and  $\text{HoBa}_2\text{Cu}_4^{18}\text{O}_8$ . The lines denote the linewidth in the normal state.  $T^*$  corresponds to the temperature where the pseudogap opens (after Ref. 28).

sure, and doping. Neutron diffraction experiments revealed essential information on specific interatomic distances and superexchange angles relevant for the understanding of the different types of phase transitions (structural, magnetic, metal-insulator), most prominently present in the rare-earth nickelates. The structural study of the metallization process in PrNiO<sub>3</sub> [29] profited from the



**Figure 15**

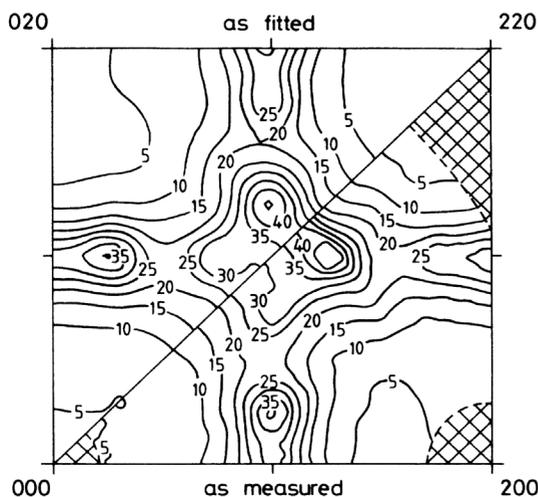
Characteristic field dependence of the magnetic excitation modes in the gapped phase of  $\text{KCuCl}_3$  at  $T=2$  K. The application of a magnetic field (3T, 5T, 6T, 14T) splits the singlet-triplet transition (ZF) into three modes (after Ref. 32).

development of a zero-matrix pressure cell allowing pressures up to 5 GPa. An interesting oxygen isotope effect was detected for the magnetic structure of the compound  $(\text{La}_{0.25}\text{Pr}_{0.75})_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ ; the sample with the isotope  $^{16}\text{O}$  is ferromagnetic, while the sample with the isotope  $^{18}\text{O}$  displays antiferromagnetic ordering [30]. The pressure-induced structural phase transition observed for the compound  $\text{Pr}_{1-x}\text{La}_x\text{NiO}_3$  and the corresponding change of the crystal-field ground state verified by neutron spectroscopy was the basis for the first experimental demonstration of cooling by adiabatic pressure application [31].

Detailed neutron scattering studies of novel **quantum spin systems** were initiated

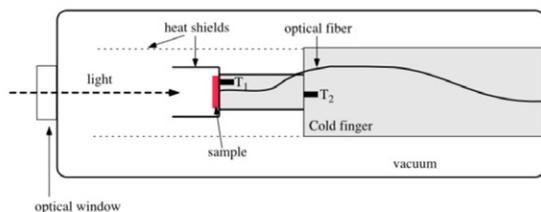
on the compound series  $\text{ACuCl}_3$  ( $A=\text{K}, \text{Ti}, \text{NH}_3$ ) which are characterized by antiferromagnetically coupled copper dimers. The resulting triplet nature of the excitations was confirmed by the observed three-fold splitting of the modes in a magnetic field as shown in Fig. 15 [32].

Investigations on a series of binary metal systems were carried out to determine **short-range order** effects by diffuse neutron scattering measurements, which provide information on the effective pair potentials. The experimental strategy was to collect a complete set of diffuse scattering data, preferably covering the irreducible part of the Brillouin zone, as exemplified in Fig. 16 for  $\alpha$ -brass [33].



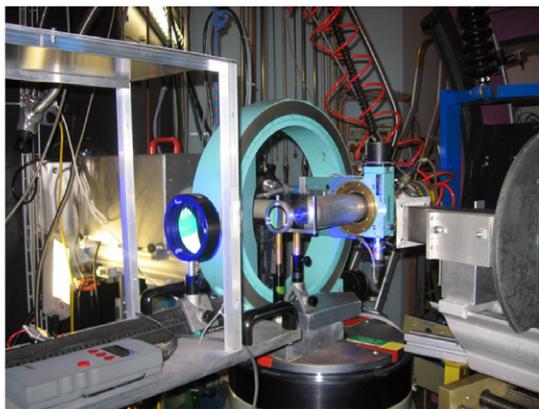
**Figure 16**

Diffuse elastic scattering observed for  $\alpha$ -brass in the reciprocal (001) plane. Experimental results (as measured) are compared with model calculations (as fitted). The lines correspond to diffuse scattering with equal intensity (after Ref. 33).



**Figure 17**

Setup for light irradiation of a single crystal of sodium nitroprusside to create maximum population of its longliving metastable states at low temperatures. These states may be controlled by measuring the transmission by means of the optical fiber connected to a photodiode situated outside the cooling system at room temperature. The photo shows this optical setup mounted on the 4-circle neutron diffractometer TriCS at SINQ.



The application of **polarized laser light for 4-circle neutron diffraction measurements on single crystals at low temperatures** was successfully developed, starting from a previ-

ously discussed experimental setup [21]. With this technique shown in Fig. 17, precise data sets of neutron intensities were collected on a single crystal of sodium nitroprusside

$\text{Na}_2\text{Fe}(\text{CN})_5\text{NO} \cdot 2\text{D}_2\text{O}$  at 80 K, both in the ground state and in a mixed state of ground state and a long-living excited state [34]. From the derived crystal structures evidence was obtained that the light-induced metastable

state differs from the ground state by distinct modifications of the Fe-N-O bond. The system has proven to be a promising material for optical storage on the molecular level.

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M. Guillaume, P. Allenspach, W. Henggeler, J. Mesot, B. Roessli, U. Staub, P. Fischer, A. Furrer, and V. Trounev  
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## 6. A glance into the 21st century

The performance of the spallation neutron source SINQ was gradually improved since its first operation, exceeding a thermal neutron flux of  $10^{14}$  n·cm<sup>-2</sup>·s<sup>-1</sup> for the first time in the year 2000. In addition, the instrumental park was continuously extended, including also world-class radiography stations. The real strength of SINQ lies on the cold neutrons rather than on the thermal ones due to the optimum placement of the cold D<sub>2</sub> source in the moderator tank. As a consequence cold neutron instruments at SINQ are often competitive with corresponding instruments at high-flux neutron sources, so that novel classes of neutron scattering experiments become possible which could hardly be carried out with use of the Swiss installations available in the 20th century. Among the many highlights resulting from experiments at SINQ in the new millennium we present below some examples of topics which were already tackled in the nineties, but came to fruition shortly after the year 2000.

The magnetic ground state of CuB<sub>2</sub>O<sub>4</sub> is incommensurate at low temperatures and undergoes a continuous phase transition to a noncollinear commensurate antiferromagnetic state at  $T^* \approx 10$  K. Coexistence of long- and short-range magnetic order is observed in both phases which suggests that the association of the Dzyaloshinski-Moriya interaction and anisotropy leads to the formation of a **magnetic soliton lattice** [35].

Below the ferro-quadrupolar ordering temperature  $T_Q = 6.1$  K of HoB<sub>6</sub> high-resolution neutron diffraction measurements on HRPT clearly detected at high scattering angles a structural

phase transition from the cubic space group *Pm-3m* to a rhombohedrally distorted structure with space group *R-3m*. The corresponding angle  $\alpha$  increases from 90 to 90.26 degrees at  $T = 2.1$  K which is clearly related to the ferro-quadrupolar ordering of HoB<sub>6</sub> [36].

The vortex lattice in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> was investigated by SANS experiments which revealed a crossover from triangular to square coordination with increasing magnetic field [37]. The existence of an intrinsic **square vortex lattice** was never observed so far in high- $T_c$  superconductors and is indicative of the coupling of the vortex lattice to a source of anisotropy, such as that provided by a d-wave order parameter or the presence of stripes.

**Chiral fluctuations** in a noncentrosymmetric crystal of MnSi were observed by using polarized neutron spectrometry, but without disturbing the sample by a magnetic field [38].

Based on the previous work on novel quantum spin systems [32], the first observation of the **Bose-Einstein condensation** in a magnetic material was reported for TlCuCl<sub>3</sub> at a critical magnetic field, where the energy of the lowest triplet component intersects the ground-state singlet, resulting in a field-induced magnetically ordered state [39].

An effort was made to search for the origin of the biquadratic exchange interaction reported for CsMn<sub>x</sub>Mg<sub>1-x</sub>Br<sub>3</sub> in earlier experiments (see Ref. 15). Among the many possible explanations, **exchange striction** turned out to be the proper mechanism [40]. This effect is commonly applied in submarine telephony and also explains the permanent hum of a transformer's iron core, as highlighted in *Physics Today* 57 (issue 8, August 2004, p. 11).

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B. Roessli, J. Schefer, G. A. Petrakovskii, B. Ouladdiaf, M. Boehm, U. Staub, A. Vorotinov, and L. Bezmaternikh, *Phys. Rev. Lett.* **86**, 1885 (2001)
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R. Gilardi, J. Mesot, A. Drew, U. Divakar, S. L. Lee, E. M. Forgan, O. Zaharko, K. Conder, V. K. Aswal, C. D. Dewhurst, R. Cubitt, N. Momono, and M. Oda, *Phys. Rev. Lett.* **88**, 217003 (2002)
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Ch. Rüegg, N. Cavadini, A. Furrer, H.-U. Güdel, K. Krämer, H. Mutka, A. Wildes, K. Habicht, and P. Vorderwisch, *Nature* **423**, 62 (2003)
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Th. Strässle, F. Juranyi, M. Schneider, S. Janssen, A. Furrer, K. W. Krämer, and H. U. Güdel, *Phys. Rev. Lett.* **92**, 257202 (2004)

## 7. Concluding remarks

The scientific highlights presented in the preceding sections are to a large extent the result of neutron scattering experiments performed at the medium-flux reactors Saphir and Diorit with thermal neutron fluxes around  $10^{14}$  n·cm<sup>-2</sup>·s<sup>-1</sup> which is an order of magnitude below the flux of the worldwide leading neutron sources. Nevertheless, the work performed at Würenlingen/Villigen turned out to be absolutely competitive on an international level and repeatedly touched innovative frontiers of condensed-matter science. The reason for these achievements is clear. The neutron source is only the first element of a usable facility, but its power can be dramatically enhanced by optimizing the instrumentation. This was made possible in Switzerland by a reasonably good level of funding and most importantly by clever staff members assisted by expert technicians who persistently tried to incorporate innovative ideas into the instruments with the aim to transport as many useful neutrons as possible to the detector.

The excellent conditions offered at Würenlingen/Villigen attracted a large national user community to perform joint experiments in the fields of crystallography, solid-state phys-

ics, chemistry, and materials science, thereby establishing the world's strongest per capita national research community in neutron scattering [41]. There were almost no administrative hurdles in the allocation of beam time, i.e., the users usually got rapid access to the instruments whenever their research programmes required neutron beams. Unfortunately, instruments for soft-matter research could not be provided due to the lack of cold neutrons. Early plans to install a cold-neutron guide hall at the reactor Saphir were given up in favor of the spallation source SINQ which concentrates on cold neutrons and therefore offers experimental possibilities in new fields of research. These new opportunities have been fully exploited by the Swiss user community. Indeed, an expert commission of the European Union made the following statement on the proposal "Access to the Neutron Scattering Facility SINQ" in the year 2001: "Recent scientific highlights listed in the proposal are impressive in both quality and range of topics covered." We therefore realize with pleasure that the tradition of neutron scattering at Würenlingen/Villigen established in the 20th century has been taken over and further developed in the 21st century up to the present.

[41] Analytical report

T. Riste, in *Neutron beams and synchrotron radiation facilities* (OECD Megascience Forum, Paris 1994), p. 63 (ISBN 92-64-14249-5)

# Design of the Bifrost spectrometer for ESS

**Jonas O. Birk<sup>1,5</sup>, Márton Markó<sup>5,2</sup>, Paul G. Freeman<sup>3,4</sup>, Felix Groitl<sup>5,3</sup>, Henrik M. Rønnow<sup>3,1</sup>, Niels B. Christensen<sup>6</sup>, Kim Lefmann<sup>1</sup> and Christof Niedermayer<sup>5</sup>**

<sup>1</sup>Nano Science Center, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark

<sup>2</sup>Neutronspectroscopy department, Wigner Research Centre for Physics, Konkoly Th. M. 29-33, 1122 Budapest, Hungary

<sup>3</sup>Laboratory for Quantum Magnetism, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

<sup>4</sup>Jeremiah Horrocks Institute, University of Central Lancashire, United Kingdom.

<sup>5</sup>Laboratory for Neutron Scattering & Imaging, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

<sup>6</sup>Institute of Physics, Technical University of Denmark, DK-2800-Kgs. Lyngby, Denmark

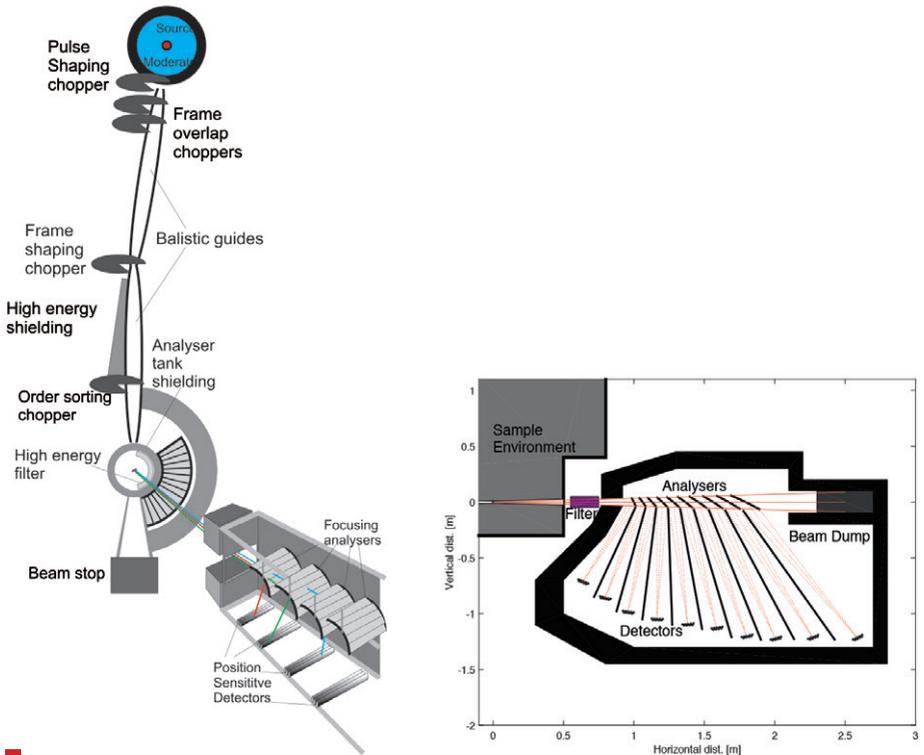
February 22, 2016

## Abstract

The European Spallation Source[17] (ESS) will become the world's leading neutron source. This is both due to the possibilities of the long pulse of the source and the many ambitious instrument concepts derived for this source. Bifrost[18, 4] is one such neutron spectrometer. Developed in a Swiss-Danish consortium it is designed to achieve a record high efficiency in the horizontal scattering plane. This will open completely new possibilities in measurements of low dimensional systems and experiments which requires extreme sample environments. The design work has led to a number of other instruments with similar Continuous Angle Multiple Energy Analysis (CAMEA) back-ends being constructed. One of these is an upgrade of RITA II[5] at PSI.

## CAMEA - Taking multiplexing to a new level

Neutron spectroscopy provides unique insight in the 4 dimensional momentum-energy space ( $q, \omega$ ) combined with the usual neutron advantages such as complicated sample environments. The technique is however flux limited. Thus resolution requirements in addition to the multi-dimensional space of interest means, that measurements can be very slow.



**Figure 1**

Schematics of Bifrost. Left: Overview of the entire instrument. Right: Side view of the analyzer-detector tank.

This is even more the case for parametric studies of for example fields, pressure, temperature, time, or a combination of these, where the parameters of interest increase the dimensionality of the investigated space. Much effort has therefore gone into improving the efficiency of neutrons spectrometers since the original triple axis spectrometer (TAS) were developed. The time-of-flight (ToF) spectrometers[23, 16, 22] have been developed and offer excellent possibilities for mapping out

large areas in  $(q, \omega)$  space simultaneously, though the drawback is a much lower intensity in each point. Contrary many TAS instruments now have the option of focusing both monochromators and analysers[11, 7], thus relaxing the  $q$ -resolution considerably but achieving higher count rates. Another approach is multiplexing, where a number of points in reciprocal space are measured simultaneously by different analyzer/detector modules. This enables traditional TAS resolution and effi-

ciency while allowing local mapping to be performed faster[10, 19, 21, 9, 7]. CAMEA can be seen as an attempt to take multiplexing to a new level, recording 3,000 - 100,000 points in  $(q,\omega)$  space simultaneously with TAS like efficiency and resolution.

The increased intensity of ESS and much higher coverage enables routinely mapping of the scattering plane of sample volumes below  $1\text{ mm}^3$ , currently too small for full neutron spectrometry. This will enable measurements of many novel materials much earlier in the synthesis process, making the process of finding materials with interesting properties much faster. The smaller samples will also enable more extreme sample environments. In particular pressure experiments will benefit from this. For example in the field of geoscience, where better understanding can be expected of the layout and dynamics further down in the earth's upper mantle and in particular the influence of water could be better understood. The much faster data acquisition will also be of great use in parametric studies. In particular time resolved studies, where it is not possible to fast forward to a few points of relevance but one has to record the entire time spectra with equal statistics. The foreseen  $< 20\ \mu\text{s}$  time resolution will be very useful for pulsed magnets but also many relaxation processes in stroboscopic measurements.

Apart from Bifrost several implementations of CAMEA have been undertaken. PSI is upgrading RITA II with a CAMEA back-end. Furthermore HZB and FRM II[13] are constructing CAMEA like instruments while ILL, HIFR and SNS strongly consider CAMEA-like instruments.

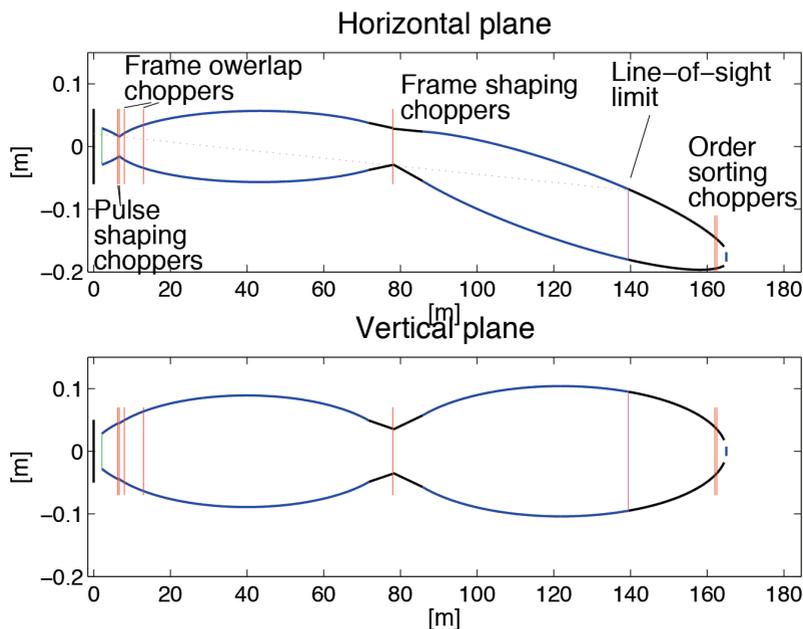
## Bifrost instrument design

The Bifrost design was performed by a Swiss-Danish consortium with partners at PSI, EPFL, Copenhagen University and the Technical University of Denmark. Since Bifrost is a completely new instrument concept considerable resources went into both design and proof of concept. The later was mainly done by a prototype, installed at MARS, PSI.[15]

Bifrost will be a cold neutron spectrometer. A bi-spectral extraction system[8] was considered but discarded, since it would have a huge impact on the most important cold spectrum if the first super mirror should fail due to radiation damage from the moderator, which is only 2m away. The cold ESS moderator is however somewhat under-moderated so measurements with energies up to  $E_i \sim 80\text{ meV}$  can be performed.

The instrument is designed for high flexibility, allowing users to pick the compromise between flux and resolution most suitable to their experiments. In the maximal flux setting the sample will be exposed to the full width of the ESS pulse, giving an  $E_i$  resolution of  $\Delta E_i/E_i = \sim 4\%$  as well as a divergence of  $\pm 0.75^\circ$  horizontal and  $\pm 1.5^\circ$  vertical. This will give a record high flux on sample of up to  $\sim 2 \times 10^{10}$  neutron/s/cm<sup>2</sup> in a  $1.7\text{ \AA}$  long bandwidth<sup>1</sup>. It is possible to reduce the divergence by the use of divergence jaws, as known from WISH[3] at ISIS and select  $E_i$  resolutions down to  $\Delta E_i/E_i = 0.1\%$  with the use of

<sup>1</sup>Since the design a number of key parameters at ESS have changed meaning that the instrument is now foreseen to be slightly shorter, with higher flux and broader bandwidth, though slightly coarser  $E_i$  resolution. This will however not change the general principles in the design.



**Figure 2**

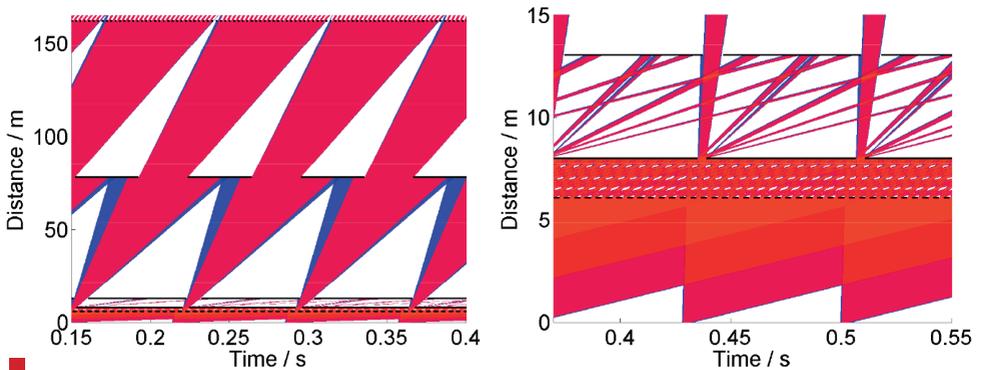
The Bifrost guide. (top) top view, (bottom) side view.

choppers, if the resolution in  $q$  and/or  $E_i$  are more important than the maximum flux.

In order to achieve the desired flexibility in resolutions and flux, the instrument is placed at 165 m from the source. This is called the natural length, since it is the shortest distance where flexible resolution can be obtained in the entire time frame without use of Wavelength Frame Multiplication[20]. The guide will be a double elliptical guide with a kink between the two ellipses. The kink ensures that direct line-of-sight to the moderator is lost 25 m before the sample, removing the fast neutron background while the brilliance transfer is kept at 85 - 95 % for all wavelengths of interest. McStas[12] and guide\_bot[1] were used to optimize the super mirror guide and

McStas was used to optimize the  $m$ -values, describing the mirror quality of the guide segments. Most segments now have  $m$ -values of 2.0 or less, while specific regions have  $m$ -values up to 3.5.

The chopper system contains a pulse shaping chopper pair as close to the moderator as possible (6.5 m). These choppers will determine the  $E_i$ -resolution. Two choppers will remove higher order pulses to reduce the background, and one chopper will shape the beam to avoid frame overlap. Finally, a set of order sorting choppers are planned. This chopper set will be placed shortly before the sample and will enable the instrument to distinguish first and higher order scattering from the analyzers. The order sorting choppers can be



**Figure 3**

Time-of-Flight diagram, showing the chopper cascade of Bifrost. The red is the main pulse of ESS, and the blue the tails of the pulse. A zoom of the first 15 m (right) shows how all higher order pulses (up to  $\lambda = 150 \text{ \AA}$ ) are blocked

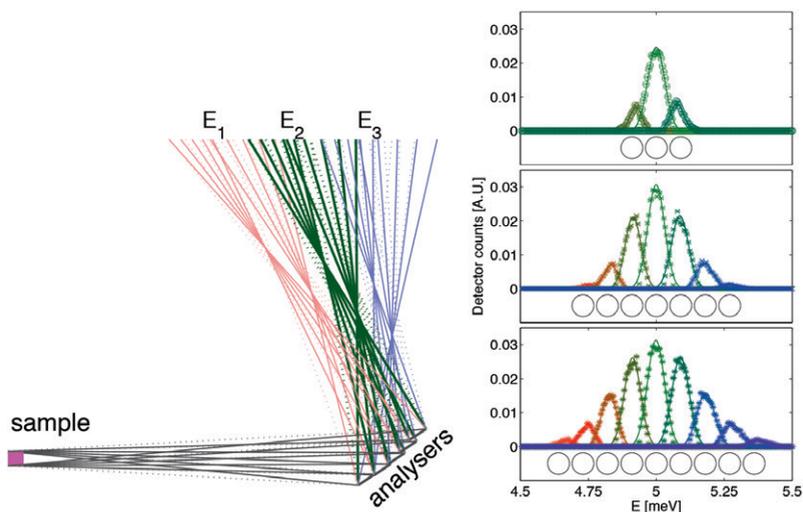
stopped and a beryllium filter used if only low energies are relevant to the experiment. After the sample the scattered neutron energy is determined by analyzer crystals[2]. The main advantage of analyzer crystals is the several hundred times higher count rate in each point in  $(q, \omega)$  space compared to direct ToF, while the main disadvantage is that the extra axis puts severe geometrical restrictions on the simultaneously measurable points. CAMEA maximizes the measured scattering in the horizontal scattering plane, to match the visible arc in many sample environments like split coil magnets and pressure cells. To maximize the angular coverage the analyzers are arranged in arcs that reflect neutrons to detectors below the scattering plane in a way that resembles Flatcone[9] at ILL. However due to the use of long analyzer crystals and

position sensitive detectors it is possible to achieve a finer angular resolution. The analyzer crystals are vertically focusing to achieve the best possible energy resolution and increase the signal to noise ratio. As every analyzer only reflects a narrow wavelength band and is almost transparent for cold neutrons not fulfilling Braggs law, several layers of analyzers can be placed behind each other, reflecting different energies to different detectors. Pyrolytic graphite crystals are used as they have the highest reflectivity as well as best transmission of non-reflected neutrons (98% for cold neutrons).

## Prismatic analyzers

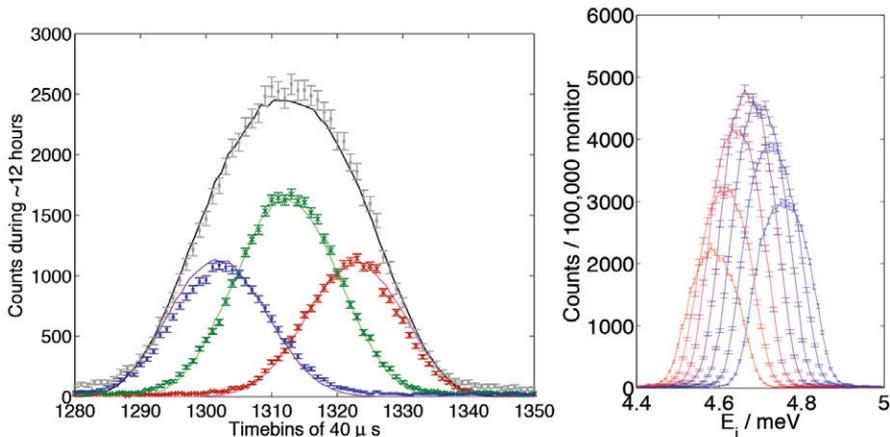
A truly novel concept in Bifrost is the Prismatic Analyzers. These take advantage of constantly smaller samples required in neutron spectroscopy, whether this is due to challenges of producing large crystals, sample environment requirements or in some cases absorption issues. While smaller samples reduce the count rates they do also provide new possibilities. If combined with small detectors, the geometrical constraints on the possible scattering paths from sample via analyzer to detector (named distance collimation) will provide a finer energy res-

olution than usually achieved from the mosaicity of analyzer crystals. A finer energy resolution is not necessarily an advantage as it also reduces the statistics, however a smaller detector does not change the amount of scattered neutrons. Thus, it is possible to collect the other neutrons in other detectors and thus achieve a finer energy resolution with no cost in flux. Furthermore, it is possible to relax the mosaicity, which both decrease the cost and increase the amount of scattered neutrons (see figure 4). The resolution is still determined by distance collimation so the full effect of the prismatic analyzers are a better



**Figure 4**

Left: Illustration of how 3 different wavelengths are reflected in 3 different directions from a focusing analyzer. Right: Each peak in the left column shows simulated counts in a single detector tube as function of  $E_i$  (The detector tubes are represented by circles below the data). The mosaicity of the analyzer is 25' (top), 60' (middle), and 90' (bottom). Modified from [2]



**Figure 5**

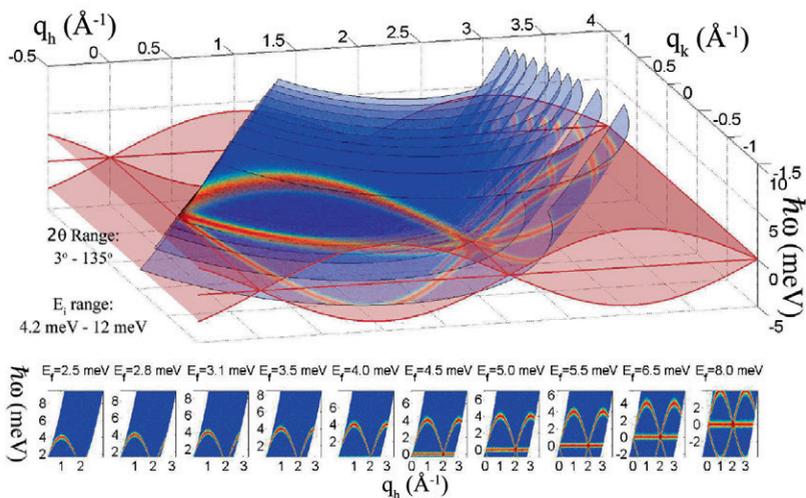
Left: Prismatic analyzers tested on the Bifrost prototype. Simulated (lines) and prototype (crosses) data of three 0.5 inch  $^3\text{He}$  tube detectors recording data from 5 analyzers arranged in a Rowland geometry. Data are taken on a Vanadium sample and kept in original time bins. The simulated data have been rescaled with a common intensity renormalization factor. The gray line shows a sum of the 3 signals and represent what would be seen in a traditional setup with a single detector. Right: Prismatic analyzers tested at TASP, PSI. A narrow slit was placed in front of the detector and energy scans of the elastic line in Vanadium were performed with different slit positions. The different detector positions are represented by different colors and lines represent Gaussian fits. Modified from [2]

energy resolution and higher total recorded flux compared to a traditional analyzer setup.

The system can be used in a focusing Rowland geometry to increase the solid angle covered by analyzers and works both in indirect ToF, where ToF is used to determine  $E_i$ , and more traditional TAS setups (see figure 5).

## Bifrost performance

Bifrost will altogether have 15 analyzer-detector modules with each  $6^\circ$  horizontal coverage and  $3^\circ$  dark angles in between. With a possible angular resolution of  $\sim 0.5^\circ$  this corresponds to  $\sim 180$  different resolvable data points. Each module will have 10 analyzer groups behind each other reflecting 10 different wavelength bands to the detectors (see figure 1). Here they will be split into 30 different energies by the prismatic analyzer concept (60, if order sorting choppers are used see figure 3). At the incoming side the indirect ToF

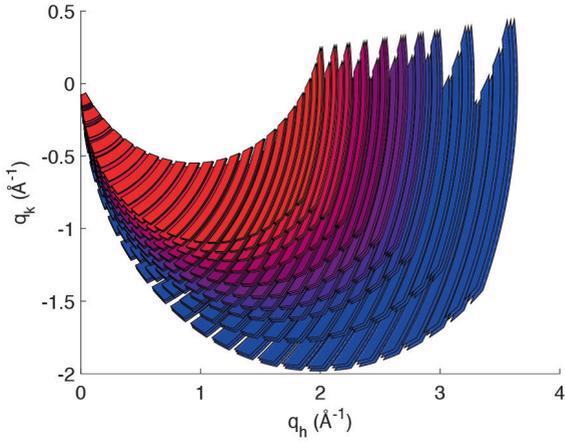


**Figure 6**

Illustration of data from a single CAMEA data acquisition. Data from a sample with an incoherent elastic line and a magnon dispersion in a low dimensional system is displayed. The simulation is done for the full ESS pulse. For clarity only 10 surfaces, corresponding to 10 analyzer-detector groups are shown and displayed below. When including the 3 energies from each analyzer, the number would be as high as 30 (60 when including the order sorting chopper). Dark angles are omitted. From [4]

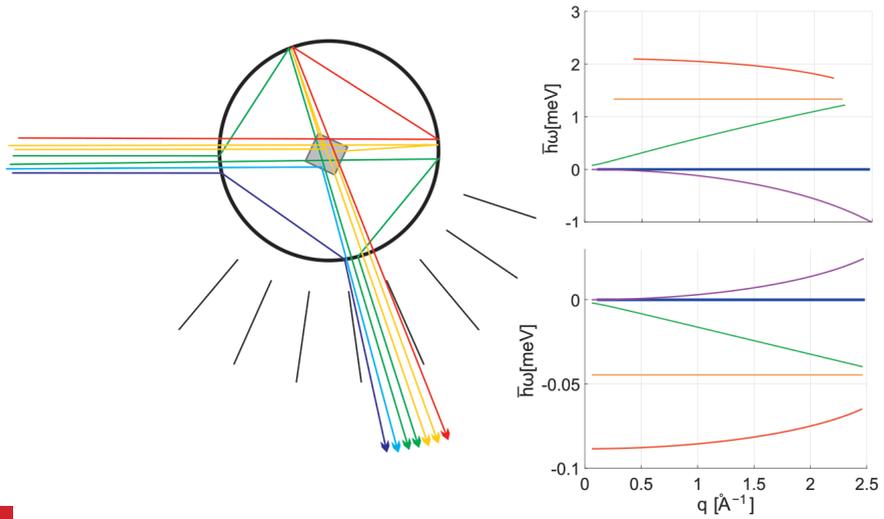
will ensure that the  $1.7\text{\AA}$  wavelength band will be resolved in at least 30 different  $E_i$  values depending on the chosen resolution. Combined this means that more than 100,000 points in  $(q, \omega)$  space will be resolved simultaneously. Figure 6 shows an example of how these points could be used to measure a magnon dispersion plus an elastic incoherent line. In this case the energy resolution is calculated in the maximum flux setting and the dark angles are covered by conducting two measurements with slightly rotated detector-analyzer modules. As it can be seen many experiments can be performed without rotating the sample at all. If the sample is

rotated the area in between the manifolds will also be covered, corresponding to a continuous covered 3 dimensional subspace of  $(q, \omega)$ . If the sample is rotated most dark angles will be covered by other analyzers (see figure 7). Compared to direct ToF spectrometers at ESS, Bifrost will have up to  $\sim 20$  times higher count rates in the horizontal plane or comparable count rates, if the direct ToF spectrometer can utilize its full  $\pm 30^\circ$  vertical coverage. Direct ToF does however enable higher resolution flexibility and will thus often be preferable, if more than the horizontal scattering plane is of interest.



**Figure 7**

Example of the elastic plane coverage of BIFROST when the sample is rotated 30°. Red indicate analyzers with low energies and blue those with higher energies.



**Figure 8**

Certain multiple scattering paths cannot be shielded by external collimation. In a simple model with a single cylinder of sample environment and a sample 6 such paths can be realized with 2 scattering events (Left). The different travel distance leads to wrong energy determination. For  $E_f = 5$  meV elastic scattering and a very large 45 cm radius sample environment this will lead to background lines in  $(q, \omega)$  as indicated. Right top: Direct ToF with 4 m secondary flight path. Right bottom: Indirect ToF with 160 m primary flight path (Bifrost).

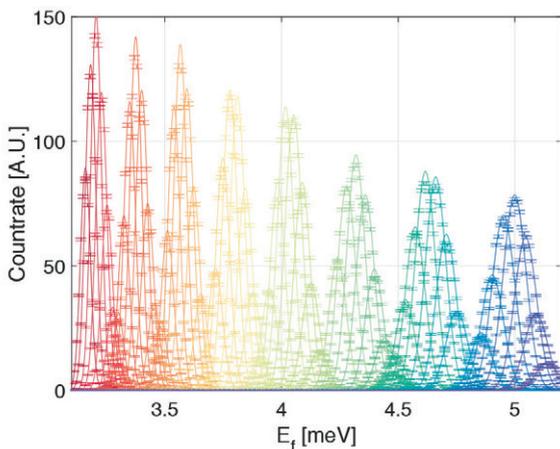
## Background

Obtaining a low inelastic background is crucial for the success of any spectrometer. In the CAMEA case the impact of sample environments on the background is especially important. Thus, a number of steps have been taken to reduce the background to a very low level. The guide is bent out of line of sight to reduce the high energy neutron background to a minimum. Recent studies show that this together with the instrument position 165 m away from the source makes it possible to obtain a fast neutron background below the cosmic background.[14] Slits and the divergence control system will limit the non-useful neutrons that reach the sample area. In addition, the sample jaws will reduce the visible area above and below the sample and a radial collimator will shield off sample environments in the sample plane. Between the analyzers and detectors the neutrons are led through vanes with absorbing sides, efficiently blocking any crosstalk between detectors and analyzers. The analyzer/detector tank will be in

vacuum to remove air scattering and all non-active components will be shielded by neutron absorbing materials. Prototype measurements suggest that this will lead to an inelastic background of  $5 \times 10^{-5}$  as compared to the elastic line of Vanadium. Furthermore, the inverse ToF setup means, that scattering from the sample environments that passes the radial collimator will be contained within the instrumental resolution of the elastic line whereas it can cause spurious signals up to 30% away from the line in direct ToF (see figure 8).

## RITA II

A CAMEA upgrade of the secondary spectrometer is currently under construction at RITA II, PSI.[6] Here, the reflected energies from the 8 analyzers will be chosen closer together, giving a quasi-continuous energy coverage of  $3.1 \text{ meV} < E_f < 5.2 \text{ meV}$  (see figure 9). Thus, in some cases it will be possible to perform full



**Figure 9**

Simulation of the raw data from energy scans, giving the resolution of the CAMEA upgrade for RITA II, PSI.

energy scans in a single acquisition with triple-axis intensities. It will have a 90° angular coverage with up to 50% dark angles for the lower energies. The upgraded spectrometer will increase the  $(q,\omega)$  coverage of RITA II from 9 to ~ 3000 points, with better  $E_f$  resolution and comparable  $q$ -resolution. When upgraded RITA II will become a world leading local mapping spectrometer and experiences gained here will benefit the construction of Bifrost of ESS.

## Conclusion

The CAMEA concept promises to be an extremely powerful secondary spectrometer. Implemented at an inverse time-of-flight spectrometer at ESS it will enable mapping of large subspaces of  $(q,\omega)$  with very high efficiency and low inelastic background.

During the design the new Prismatic Analyzer concept was developed. This concept allows measurements with finer resolution and higher total count rates simultaneously than comparable crystal analyzer spectrometers.

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# Announcements

## SGN/SSDN Members

Presently the SGN has 200 members. New members can register online on the SGN website: <http://sgn.web.psi.ch>

## SGN/SSDN Annual Member Fee

The SGN/SSDN members are kindly asked to pay their annual member fees. At the general assembly 2013 of the society, the fee has been increased from CHF 10 to **CHF 20**. It can be paid either by bank transfer or in cash during your next visit at PSI. The bank account of the society is accessible for both Swiss national and international bank transfers. The coordinates are as follows:

Postfinance: 50-70723-6 (BIC: POFICHBE),  
IBAN: CH39 0900 0000 5007 0723 6.

The SGN is an organization with tax charitable status. All fees and donations paid to the SGN are **tax deductible**.

## PSI Facility News

Recent news and scientific highlights of the three major PSI user facilities SLS, SINQ and  $\mu\text{S}$  can be found in the **quarterly electronic newsletter** available online under: <https://www.psi.ch/science/facility-newsletter>

## 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>) is: **May 15, 2016**

## Registration of publications

Please remember to **register all publications either based on data taken at SINQ, SLS,  $\mu\text{S}$  or having a PSI co-author** to the Digital User Office: <https://duo.psi.ch>. Please follow the link 'Publications' from your DUO main menu.

## Open Positions at SINQ and ILL

To look for open positions at SINQ or ILL, have a look at the following webpages:  
<https://www.psi.ch/lbr/open-positions>  
<http://www.ill.eu/careers>

## PhD positions at ILL

The PhD program of the Institut Laue-Langevin, ILL, is open to researchers in Switzerland. The contact person at ILL is Anne-Claire Dupuis (PhD@ill.eu). The Swiss agreement with the ILL includes that ILL funds and hosts one PhD student from Switzerland

# Conferences and Workshops 2016 and beyond

An updated list with online links can be found here:  
<http://www.psi.ch/useroffice/conference-calendar>

## March 2016

80th Annual Meeting and Spring Meeting of the German Physical Society (DPG)  
 March 6-11, 2016, Regensburg, Germany

Fourth training course on symmetry and group theory | March 7-11, 2016, Tsukuba, Japan

9th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples  
 March 9-11, 2016, Lund, Sweden

24th Annual Meeting of the German Crystallographic Society (DGK) | March 14-16, 2016, Stuttgart, Germany

ISIS Muon Training School 2015  
 March 14-18, 2016, ISIS facility, Abingdon, UK

HERCULES 2016 - European School  
 March 29 - April 29, 2016, Grenoble, France

2nd International Conference on Image Analysis in Three-dimensional Cryo-EM  
 March 30 - April 2, 2016, Lake Tahoe, CA, USA

## April 2016

Erice School on Neutron Science and Instrumentation: Designing and Building a Neutron Instrument | April 1-9, 2016, Erice, Sicily, Italy

Magnetism 2016  
 April 4-5, 2016, Sheffield, UK

BCA Spring Meeting  
 April 4-7, 2016, Nottingham, UK

9th COST School on Surface Analytical Techniques | April 4-7, 2016, Regensburg, Germany

- Macromolecular Crystallography School 2016: From Data Processing to Structure Refinement and Beyond | April 4-13, 2016, Sao Carlos, Brazil
- Understanding Complex Macromolecular Systems from Sparse Data: The Astbury Conversation | April 11-12, 2016, Astbury Centre at the University of Leeds, UK
- SCTE2016: 20th Conference on Solid Compounds of Transition Elements  
April 11-15, 2016, Zaragoza, Spain
- Crystallization: Focus on Micro and Nano Crystals and High Throughput Methods  
April 19-22, 2016, SLAC, Menlo Park, CA, USA
- ICSM2016: 5th International Conference on Superconductivity and Magnetism  
April 24-30, 2016, Fethiye, Turkey
- Practical X-ray Fluorescence  
April 25-29, 2016, Newtown Square, PA, USA
- Protein Structure, Dynamics and Function  
April 29 - May 1, 2016, Providence, RI, USA
- May 2016
- 24th Journées de la Diffusion Neutronique: Multidisciplinary Science with Neutrons  
May 2-4, 2016, Carqueiranne, Var, France
- CETS2016: 10th Central European Training School on Neutron Techniques  
May 2-6, 2016, Budapest, Hungary
- 2016 E-MRS Spring Meeting and Exhibit  
May 2-6, 2016, Lille, France
- Future Applications of Small-Small Angle Scattering to Soft Matter  
May 5, 2016, Swindon, Wiltshire, UK
- 7th Workshop on Neutron Scattering Applications in Structural Biology  
May 16-20, 2016, Oak Ridge, TN, USA
- Fundamentals of X-ray Powder Diffraction  
May 16-20, 2016, Newton Square, PA, USA
- Advanced Methods in X-ray Powder Diffraction  
May 23-27, 2016, Newton Square, PA, USA
- High-Pressure Crystallography: Status Artis and Emerging Opportunities - 49th Erice Course  
May 27 - June 5, 2016, Erice, Sicily, Italy
- IWTAP-2016: International Workshop on Theoretical and Applied Physics  
May 28-29, 2016, Istanbul, Turkey
- ISC Granada 2016. 5th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2016)  
May 29 - June 3, 2016, Granada, Spain
- June 2016
- COC2016: 2nd Conference on Organic Chemistry | June 1-3, 2016, Nanjing, China
- Science Summer School  
June 2 - July 13, 2016, Grenoble, France

20th Real Time Conference  
June 5-10, 2016, Padova, Italy

IWPCPS-17: International Workshop for Physical Characterization of Pharmaceutical Solids  
June 6-9, 2016, Winter Park, FL, USA

13th TOPAS User's Meeting  
June 10-12, 2016, Bari, Italy

EPDIC15: 15th European Powder Diffraction Conference | June 12-15, 2016, Bari, Italy

DRC 2016: 74th Device Research Conference  
June 19-22, 2016, Newark, DE, USA

Structural and Biophysical Methods for Biological Macromolecules in Solution  
June 19-26, 2016, Newark, Suwon, Korea

13th European Summer School on "SCATTERING METHODS APPLIED TO SOFT CONDENSED MATTER" | June 20-27, 2016, Bombannes, France

58th Electronic Materials Conference  
June 22-24, 2016, Newark, DE, USA

9th K.H. Kuo Summer School of Electron Microscopy and 2016 Kuo Symposium on 3D Cryo-EM Molecular Imaging  
June 24-30, 2016, Beijing, China

DSL2016: 12th International Conference on Diffusion in Solids and Liquids  
June 26-30, 2016, Split, Croatia

ECDM7: 7th European Charge Density Meeting  
June 26 - July 1, 2016, Warsaw, Poland

NIST Summer School on Methods and Applications of Small Angle Neutron Scattering and Neutron Reflectometry

June 27- July 1, 2016, Gaithersburg, MD, USA

International School on Fundamental Crystallography with Applications to Electron Crystallography | June 27- July 2, 2016, Antwerp, Belgium

July 2016

ICCBM-16: 16th International Conference on the Crystallization of Biological Macromolecules

July 3-7, 2016, Prague, Czech Republic

ICRS-10: 10th International Conference on Residual Stresses

July 3-7, 2016, Sydney Brighton Le Sands Beach, Australia

VUVX2016: 39th International conference on Vacuum Ultraviolet and X-ray Physics

July 3-8, 2016, Zurich, Switzerland

PNCMI: International Conference on Polarised Neutrons for Condensed Matter Investigations

July 4-7, 2016, Freising, Germany

3rd International School on Aperiodic Crystals  
July 4-8, 2016, Antwerp, Belgium

Swiss MaNEP Workshop on Quantum Materials and Electronic Devices

July 6-8, 2016, Les Diablerets, Switzerland

- ACNS 2016: 8th American Conference on Neutron Scattering | July 10-14, 2016, Long Beach, CA, USA
- August 2016
- Denver X-ray Conference. 65th Annual Conference on Applications of X-ray Analysis  
August 1-5, 2016, Rosemont, IL, USA
- SXNS14: Annual International Conference on Surface X-ray and Neutron Scattering  
July 10-14, 2016, Long Island, NY, USA
- 16th International Summer School on Crystal Growth (ISSCG-16)  
August 1-7, 2016, Shiga, Japan
- 16th IUBMB Conference  
July 17-21, 2016, Vancouver, Canada
- MH2016: 15th International Symposium on Metal-Hydrogen Systems  
August 7-12, 2016, Interlaken, Switzerland
- MLZ Conference on 'Neutrons for Energy'  
July 18-21, 2016, Bad Reichenhall, Germany
- 12th International Congress of Cell Biology  
July 21-25, 2016, Prague, Czech Republic
- 12th International Conference on Biology and Synchrotron Radiation (BSR)  
August 21-24, 2016, SLAC National Accelerator Lab., Stanford, USA
- Workshop on 'Computational Approaches to the Structural Modelling of Biological Macromolecules using Small Angle Scattering'  
July 22, 2016, Denver, CO, USA
- International Conference on Structural Biology  
August 22-23, 2016, New Orleans, USA
- Session on 'Magnetic entanglement and complex magnetic materials' during the 2016 American Crystallographic Association Meeting | July 22-26, 2016, Denver, CO, USA
- ECM-30 Satellite: Neutron Powder Diffraction School 2016  
August 22-26, 2016, Villigen, Switzerland
- Session on 'SAS and Integrative Approaches to Complex Structures' during the 2016 American Crystallographic Association Meeting  
July 22-26, 2016, Denver, CO, USA
- Joint European Magnetic Symposia (JEMS)  
August 22-26, 2016, Glasgow, UK
- SPS Annual Meeting 2016  
August 23-25, 2016, Ticino, Switzerland
- Magnetic Structure and Analysis by Neutron Diffraction Techniques  
July 22-26, 2016, Denver, CO, USA
- MPBH SINERGIA Workshop 2016: Mott Physics Beyond the Heisenberg Model  
August 23-25, 2016, London, UK
- Bunsen Discussion Meeting: Neutrons in Chemistry | July 25-27, 2016, Bielefeld, Germany

ECM-30 Satellite: International school on charge and spin electron density and derived properties: from experimental determination to interpretation

August 24-27, 2016, Nancy, France

ECM-30: European Crystallographic Meeting

August 28 - September 1, 2016, Basel, Switzerland

EMC2016

August 28 - September 2, 2016, Lyon, France

## September 2016

50 Years of Neutron Backscattering Spectroscopy

September 2-3, 2016, Garching, Germany

The 54th European High Pressure Research Group (EHPRG) International Meeting on High Pressure Science and Technology

September 4-9, 2016, Bayreuth, Germany

International Conference in Science@FELS 2016 | September 5-7, 2016, Trieste, Italy

QENS 2016: International Conference on Quasielastic Neutron Scattering

September 5-8, 2016, Berlin, Germany

WINS 2016: Workshop on Inelastic Neutron Spectrometers

September 8-9, 2016, Berlin, Germany

21st International Conference on Cyclotrons and their Applications

September 11-16, 2016, Zurich, Switzerland

ISMC 2016: 4th International Soft Matter Conference

September 12-16, 2016, Grenoble, France

Deutsche Neutronenstreutagung 2016

September 20-22, 2016, Kiel, Germany

3rd European Crystallography School (ECS3)

September 25 - October, 2, 2016, Bol, Croatia

## October 2016

MEDSI2016: Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation

October 2, 2016, Barcelona, Spain

4th International Conference on Competitive Materials and Technology Processes

October 3-7, 2016, Miskolc, Hungary

PSI2016: Physics of fundamental Symmetries and Interactions

October 16-20, 2016, PSI Villigen, Switzerland

NSS: IEEE Nuclear Science Symposium 2016

October 29 - November 6, 2016, Strasbourg, France

## June 2017

muSR2017: International conference on mu-SR spectroscopy

June 25-30, 2017, Sapporo, Japan

## July 2017

ICNS 2017: 9th International Conference on  
Neutron Scattering  
July 9-13, 2017, Daejeon Convention Center,  
Korea

## August 2018

XRM2018: 14th International Conference on  
X-ray Microscopy  
August 19-24, 2018, Saskatoon, Saskatche-  
wan, Canada

## October 2018

SAS2018: XVII International Conference on  
Small-Angle Scattering  
October 7-12, 2018, Traverse City, MI, USA





## Editorial

### Editor

Swiss Neutron Scattering Society

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henrik.ronnow@epfl.ch

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Dr. M. Kenzelmann  
michel.kenzelmann@psi.ch

Dr. L.E. Bove

livia.bove@epfl.ch

Dr. U. Gasser (secretary)

urs.gasser@psi.ch

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### Address

Sekretariat SGN/SSDN  
c/o Paul Scherrer Institut  
WLGA/018  
5232 Villigen PSI, Switzerland  
phone: +41 56 310 46 66  
fax: +41 56 310 32 94  
<http://sgn.web.psi.ch>

### Bank Account

Postfinance: 50-70723-6 (BIC: POFICHBE)  
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Sekretariat SGN/SSDN  
WLGA/018  
Paul Scherrer Institut  
5232 Villigen PSI, Switzerland

