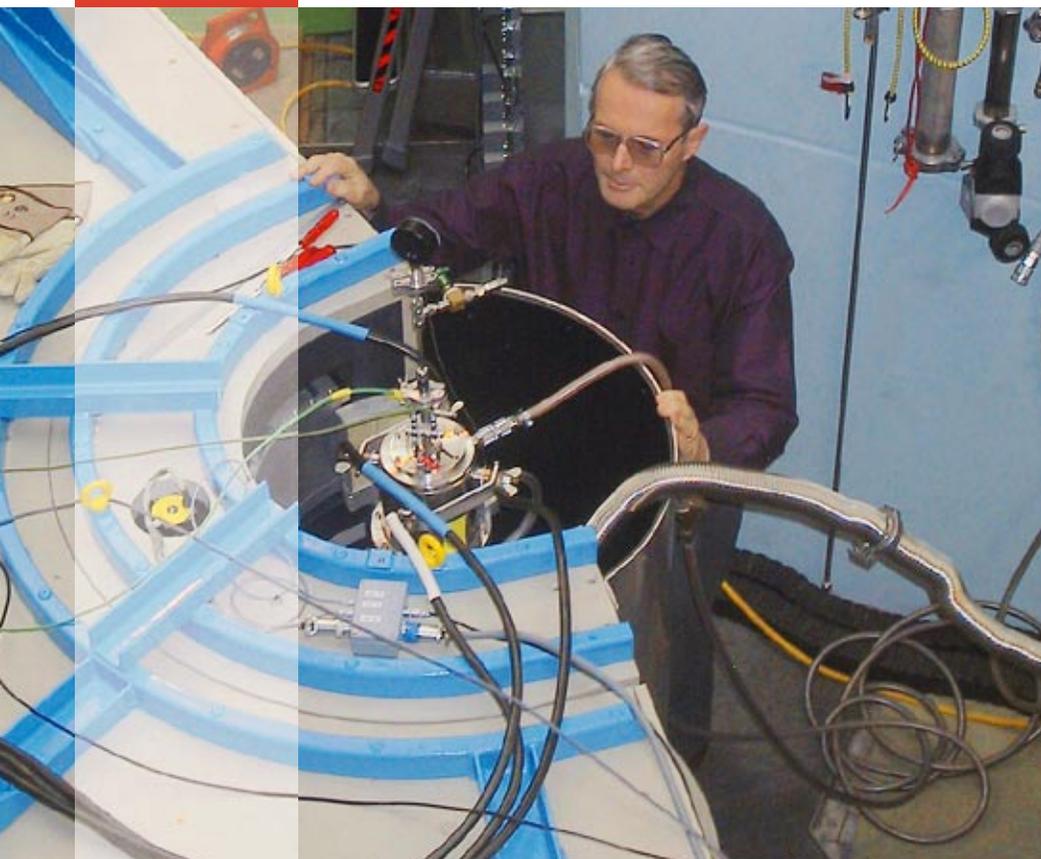


# SWISS NEUTRON NEWS



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

## Editorial

Editor: Swiss Neutron Scattering Society

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## Cover illustration

*Peter Fischer (Laboratory for Neutron Scattering, PSI & ETHZ) working at "his" high resolution powder diffractometer HRPT at SINQ. After 40 years working in the field of neutron diffraction he retired in October 2002. The Swiss Neutron Scattering Society wishes him all the best for the future.*

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## *The SGN/SSDN President's Page*



Dear members,

in the last editorial I commented on the international ESS conference on May 16–17 in Bonn and wrote that “the demonstration by the scientists was indeed impressive, and I only hope that the European decision makers do follow and support us in our strive for a leap into the next generation of large scale research facilities. The ESS certainly will be important not only for basic research, but allow us to tackle many new problems of techno-

logical and economical relevance.” Unfortunately, the Science Council of Germany (Wissenschaftsrat, WR) apparently did not share this opinion and expressed doubts about the long-term importance of neutrons. This assessment was indeed found unfair by many scientist and stirred a quite impressive series of comments and open letters from the international neutron user community that included such prominent scientists as the Nobel laureates Richard Ernst and Alex Müller. The ESS Project received broad encouragement from scientists world wide, and it is fair to say that scientists from all areas have only rarely engaged in such a public effort to demonstrate the effectiveness and future relevance of neutron research for almost all condensed matter disciplines. Moreover, the States of Sachsen/Sachsen and North Rhine Westfalia continued to hold on to their commitment to try and realise ESS, and together with ESS they elaborated the project documents in accordance with the verdict of the WR, and they resubmitted it formally for a re-assessment of the European Spallation Source.

It is clear that the ESS will be vital for the future of our community, and only with such a 3rd generation neutron source we shall be able to extend the currently accessible range of problems and tackle the most interesting and important scientific questions of the future. It is thus important that we all do our best in trying to convince the public and the politicians to recognise the crucial role played by neutron scattering in sustaining and advancing condensed matter science and technology in Europe, and to assess the importance of the ESS project in this context.

While there may be some threats on the long term future of neutron scattering in Switzerland and in Europe, it is clear that presently the science at SINQ has experienced a real boost. The demand for neutron beam time as expressed by the number of scientific proposals submitted to our national source continues to be very high. More-

over, several areas that were very active on an international scale but used to be only marginally covered at SINQ, such a soft condensed matter, now have a much larger number of proposals. I believe that this is largely a result of the participation of SINQ in the 5<sup>th</sup> EU framework program (FP5). A special thanks should go to the 'Bundesamt für Bildung und Wissenschaft, BBW', who has agreed to fund the project, since the delay of the ratification of the bilateral agreements between Switzerland and the EU had made it impossible to obtain the funding for this successful project directly from Brussels. It is clear that we all profit from this increased international attractiveness and competitiveness of SINQ. This becomes even more important in view of the fact that the successor program FP6 has not been included in the bilateral treaty, and that a renewal of this project in FP6 thus has to be renegotiated with the EU. I think it will be vital for the scientific success of SINQ to continue with this program, and I hope that the BBW will continue with their support if these negotiations will be delayed.

I think that all this has demonstrated how important it is to continue to point out to the public the importance of large scale research facilities, and in particular of neutron scattering, for the advancement of science and technology. However, it is also clear that all this is not sufficient if the we can not continue to do what our community has been so successful in doing in the past, and that is to do outstanding science. In this respect it is comforting to see that a young member of our society, Joël Mesot from the Laboratory of Neutron Scattering, PSI and ETHZ, has recently been given the highly prestigious Latsis Prize of the ETHZ for his outstanding research achievements. Congratulations!

Peter Schurtenberger

# *Forty Years of Neutron Diffraction in Switzerland*

J. Schefer

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## **In honor of Dr. Peter Fischer's 65<sup>th</sup> birthday**



**Peter Fischer**  
LNS ETHZ & PSI

Neutron scattering has a long tradition within Switzerland, which has the world strongest “per capita” national user community [1]. What is the reason? For this we have to go back to the early days of neutron sources in our country.

In 1953, a project to build the Swiss research reactor DIORIT, started in 1952 by a private consortium of 171 Swiss companies headed by Brown Boveri (BBC), Sulzer and Escher Wyss, was presented to the Swiss government. Construction was completed three years later by the Reaktor AG. The DIORIT reactor went critical on August 26, 1960. The delay in starting operation was due to a second research reactor (SAPHIR), which was acquired in parallel: This was on the initiative of Max Petitpierre, the Swiss Federal Council of Foreign Affairs, who was also President of Switzerland at the time. The reactor SAPHIR (Figure 1) was sold by the US government for only 770'000 Swiss francs, at the occasion of the exhibition *Atoms for Peace* held in 1955 at the *Palais des Nations* in Geneva. It was named SAPHIR because of the blue Cerenkov radiation in the reactor pool.



**Figure 1:** Loading the parts of SAPHIR for its journey to the Geneva exhibition “Atoms for peace” (1955).

Three goals were pursued with these new research instruments: Reactor development, training of reactor personnel and condensed matter research. The Institute for Reactor Research of the ETH Zurich, headed by Professor Walter Halg, was therefore divided into two parts: Reactor technology located in Zurich and the division *Education & Research (Ausbildung & Forschung, Delegation AF)* located in Wurenlin-

gen. In 1960, the Reaktor AG was transformed into the government owned *Eidgenössische Institut für Reaktorforschung* (EIR).



**Figure 2:** *Delegation AF (1962) in the chemistry building (today OFLC) at Würenlingen (from the left: Prof. Walter Hätig, Hans Ripfel, Peter Fischer, Georg Maier, Frans Brandt, Ferruccio Ferroni [Natrium loop]).*

Peter Fischer started his career at the ETH Zurich, where he made his Masters thesis on the properties of tin telluride, under the supervision of Professor Georg Busch. In summer 1961, he joined the *Delegation AF* in Würenlingen as a thesis student (Figure 2), together with Georg Maier. This PhD thesis on spinels  $MgAl_2O_4$  was on an initiative of Professor Fritz Laves, who was looking for a method to distinguish Al and Mg, as this was problematic with X-rays [2].

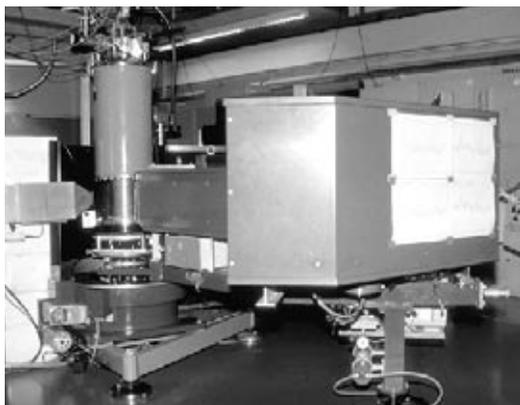
With his collaborators, he installed a spectrometer equipped with a mechanical 1:2 drive for simultaneous change of  $\omega$  and  $2\Theta$  which was based on an optical spectrometer built by the company Toepfer; the instrument was on loan from the university of Basel. It was tested at the reactor SAPHIR. Peter Fischer started to investigate the magnetic properties of MnBi in collaboration with his Norwegian teacher and friend, A.F. Andresen [3], who unfortunately died in 1991 in a car accident. The instrumentation used at the DIORIT is shown in Figure 3. He was supervisor of many future neutron scatterers such as Willi Bühner (†1997), Professor Albert Furrer, Karel Tichy, Heinz Heer and Werner von Wartburg and myself.



**Figure 3:** *Instrumentation installed at the reactor Diorit in Würenlingen.*

One thing crystallized out of all this work very quickly: Condensed matter physics will be his interest, therefore powder diffraction his method of choice to investigate new materials. This is obvious as neutrons are very valuable for investigations of bulk properties as well as of magnetism. Instrumentation and computing programs were not so well developed in those days. Peter Fischer therefore got very interested in developing new instrumentation. He was always one step ahead and particularly made sure he had the latest software installed on the newest computers. This way, he became one of the first using consequently the (new) Rietveld profile refinement method, and thereby contributed significantly to its development. Therefore it is not surprising that the single detector powder diffractometer punching data onto paper tape was just too slow for him! He pushed for the introduction of linear position sensitive detectors. As a result, the DMC spectrometer at the reactor SAPHIR was put into operation in mid 1984, financed by grants from the Swiss Science Foundation, EIR, ETH Zurich and the universities of Berne and Geneva (Figure 4, [4]). Instead of a single counter, 400 wires were now covering an  $80^\circ$  range in  $2\Theta$ . Also single crystal instruments had his interest, as for example his second instrument at SAPHIR, the P2AX (Figure 5). The younger generation may just remember this instrument from the data format containing its name in the file extension (\*.2ax), which still exists.

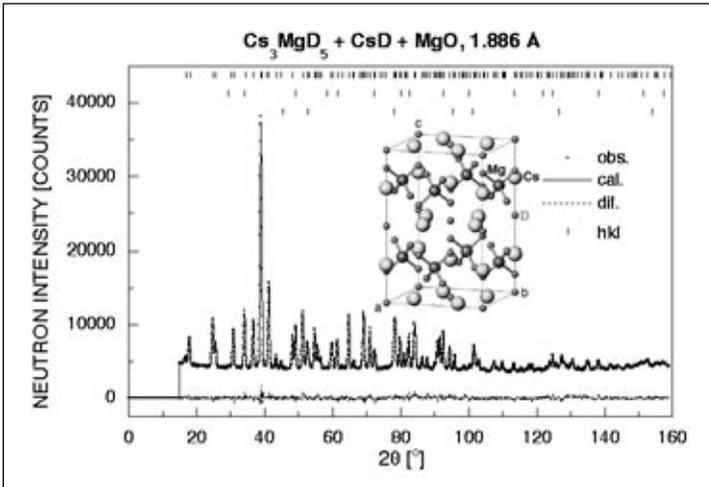
Peter Fischer was also always in the front line of new science: Hydrogen storage in metals [5], today used in many rechargeable batteries, as well as high temperature superconductors. As an example of the hydrogen storage materials, I just want to mention the magnesium based  $\text{Cs}_3\text{MgD}_5$  containing  $\text{MgD}_4^{2-}$  anions as well as  $\text{D}^-$  (bonded



**Figure 4:** Double Axis Multicounter Diffractometer (DMC) at the reactor SAPHIR. [4]. The instrument is now installed on a cold guide at SINQ.

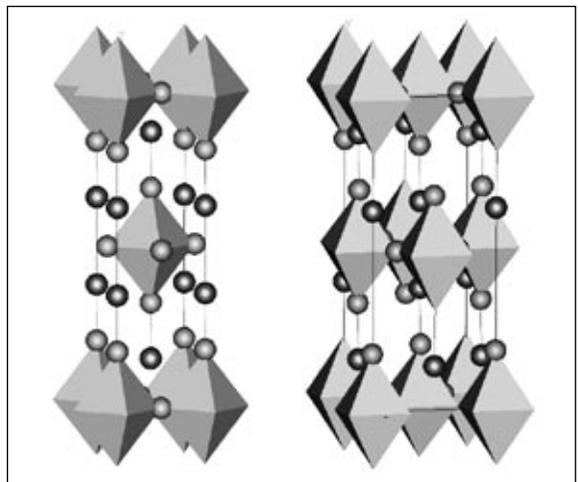


**Figure 5:** The experimental hall at the reactor SAPHIR. In the foreground the MARC spectrometer, in the center the P2AX, and in the back the single crystal and the single counter powder diffractometers.

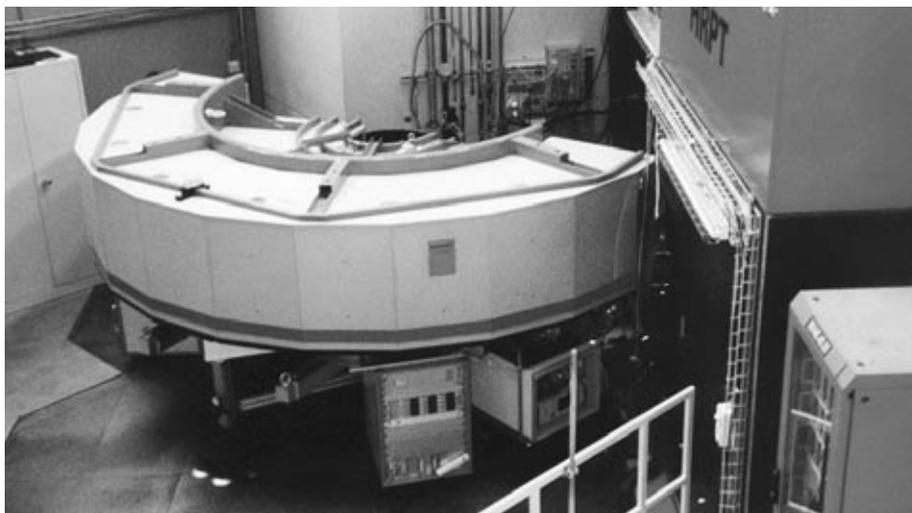


**Figure 6:** Hydrogen localisation in  $Cs_3MgD_5$ . Multi phase powder diffraction investigation at HRPT/SINQ,  $\lambda=1.886\text{\AA}$ . The additional phases are traces of CsD and MgO.

to Cs only), investigated on the HRPT at SINQ (Figure 6, [6]). In high temperature superconductors, Peter Fischer associated structural changes with superconductivity, soon after Bednorz and Müller found the effect. Together with Professor Klaus Yvon, he discovered a structural phase transition in the first high- $T_c$  material,  $(La,Sr)CuO_4$ , soon after superconductivity was reported in this material (Figure 7, [7]), and he was among the first to determine the correct structure of the  $YBa_2Cu_3O_7$  (Y123). But probably the most important work he did was with Emanuel Kaldis and Alan W. Hewat on the characterization of the  $YBa_2Cu_4O_8$  (Y124) and  $Y_2Ba_4Cu_7O_{15}$  (Y247, [8]) compound, and the study of the effect of pressure on the  $T_c$  in Y124 and Y123. This work confirmed the idea of Bob Cava and collaborators, that  $T_c$  was controlled by a charge transfer from so-called “charge reservoir” layers, and that the effect of pressure was due to the different compressibility of the superconducting and of the charge reservoir layers. We also should not forget his



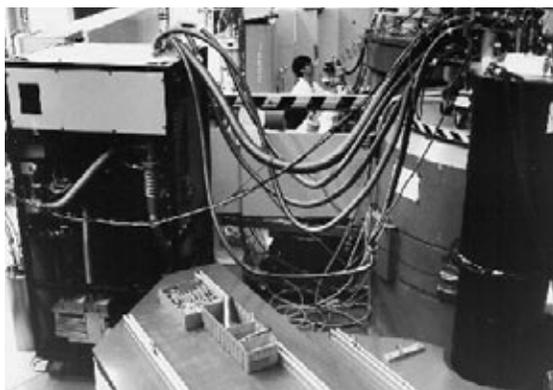
**Figure 7:** Structural phase transition in  $La_{1.85}Sr_{.15}CuO_4$  at 150K [7].



**Figure 8:** High-resolution powder diffractometer HRPT at the spallation neutron source SINQ in Villigen.

important work with his Russian colleagues on the effect of Ca substitution for Y, which changes the charge balance and therefore  $T_c$  of these materials [9] and related work with Professor Vitali Trounov. Finally, Peter worked on the magnetic structure of high-temperature superconducting materials in which Y was replaced by magnetic rare earths.

It is therefore not surprising, that Peter Fischer immediately saw the new possibilities for the Swiss neutron community when the idea of building a spallation neutron source at the proton accelerator at SIN in Villigen appeared. Of course, the “banana” detector from SAPHIR had to grow! 1600 wires are now covering  $160^\circ$  [10] at the new powder diffractometer HRPT at SINQ (Figure 8). This development from the French company CERCA with major inputs from PSI scientists and engineers (EIR and SIN merged 1988 to form PSI) was strongly pushed by Peter Fischer and went into final operation before his retirement despite facing many problems (as most pioneering work does).



**Figure 9:** The Oxford dilution refrigerator at the reactor Saphir mounted on DMC.

Another field of interest for Peter Fischer was magnetism. He always pushed (mostly successfully) to be equipped with the latest cryostats such as for example the 7 mK dilution refrigerator (Figure 9), used to study the magnetic structure of  $\text{DyBa}_2\text{Cu}_4\text{O}_8$  [11] and many other materials. He probably holds the world record concerning the ratio of successful to failed experiments in a dilution cryostat. Of course, also the “old” DMC was moving over the river, now to be installed at a super-mirror guide for cold neutrons.

The work of Peter Fischer is contained in almost 400 publications. He advised many young scientists in their Masters as well as PhD thesis work, three of them alone to be finished within this year. We thank him here on the occasion of his retirement for all his input given to science, to our group and to his colleagues worldwide. However, despite being retired, Peter Fischer will definitely not be absent from physics. We are grateful to have such an experienced “consultant” behind us.

Peter Fischer was always a member of ETH Zurich, whereas his research facilities changed it’s ownerships and names quite frequently. He officially left our institute at the end of October for his retirement. Our best wishes to him and his wife Hedi for their future. You always can reach him at [peter.fischer@psi.ch](mailto:peter.fischer@psi.ch) or at his private address, Waldweg 14, CH-5242 Lupfig.

Peter, I would like to thank you on behalf of our laboratory, but also personally, for all you have done!

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# *Metal-hydrogen complex formation*

## *in hydrogenated intermetallic compounds*

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Université de Genève, Geneva, Switzerland*

### **Abstract**

Hydrogenation of certain intermetallic compounds leads to non-metallic, colored hydrides that are nearly stoichiometric.  $\text{Mg}_2\text{Ni}$  and  $\text{Mg}_3\text{Ir}$ , for example, yield brownish  $\text{Mg}_2\text{NiH}_4$  and red  $\text{Mg}_6\text{Ir}_2\text{H}_{11}$ , respectively. Their structures and compositions can be rationalized in terms of 18-electron complexes ( $[\text{NiH}_4]^{4-}$ ,  $[\text{IrH}_5]^{4-}$ ,  $[\text{IrH}_4]^{5-}$ ) and hydrogen anions  $\text{H}^-$ , which suggests that the compounds are „complex“ rather than „interstitial“ metal hydrides. Metal-hydrogen complexes can also be discerned in metallic hydrides such as  $\text{LaMg}_2\text{NiH}_7$  ( $=\text{La}^{3+}\text{Mg}^{+2}_2 \cdot [\text{NiH}_4]^{4-} \cdot 3\text{H}^-$ ) and  $\text{NdMgNi}_4\text{H}_4$  ( $=\text{Nd}^{3+}\text{Mg}^{+2} \cdot [\text{Ni}_4\text{H}_4]^{5-}$ ) and could possibly be a general phenomenon in „interstitial“ metal hydrides, at least on a local level. This opens the door for a better understanding of metal-hydrogen interactions in metallic (interstitial) metal-hydrogen systems.

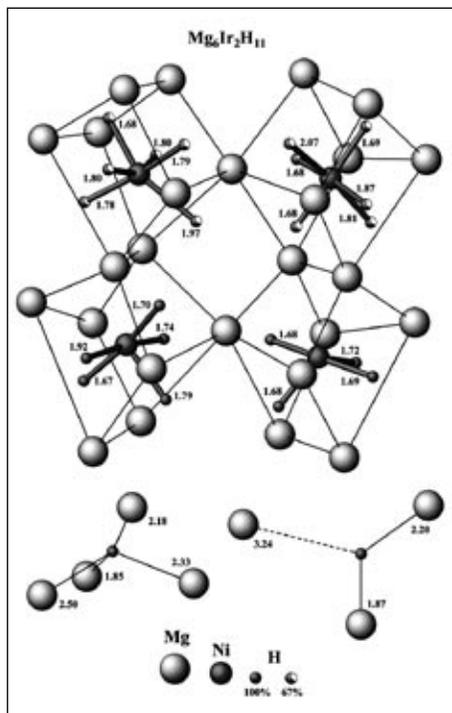
### **Introduction**

Solid-state metal hydrides provide a safe and efficient way of storing and transporting hydrogen. A fundamental aspect that needs to be better understood is the nature of the metal-hydrogen interaction and its influence on properties such as hydrogen capacity and electron localization (metal-to-nonmetal transitions). The great majority of metal hydrides known is metallic and derives from binary metal compounds [1]. They have relatively large homogeneity ranges and are usually called „interstitial“ because hydrogen occupies interstices in the metal atom network. Except for a lattice expansion and distortion the metal substructures do not much change during hydride formation. The hydrogen substructures are usually disordered at room temperature, i.e. the local hydrogen configurations around the metal atoms are unknown. A notable exception is  $\text{Mg}_2\text{NiH}_4$ . The hydride has been reported some 30 years ago, is non-metallic and derives from metallic  $\text{Mg}_2\text{Ni}$  by a relatively important rearrangement of its hexagonal metal substructure. It displays a disordered hydrogen distribution in its cubic high-temperature phase and has been originally classified as an „interstitial“ hydride. It was only after its monoclinic room-temperature structure had been solved and found [2] to contain an ordered array of tetrahedral  $[\text{NiH}_4]^{4-}$  complexes that it was classified as a so-called „complex“ metal hydride (for a recent review see [3]). The properties of the

latter are relatively well understood in the sense that their compositions and ligand geometries can be rationalized in terms of simple electron counting rules (for example the 18-electron rule) and s-p-d hybridization schemes (for example  $sp^3$ ) which is generally not possible with their „interstitial“ (metallic) counterparts. For a long time the  $Mg_2Ni-H$  system provided the only example for a hydrogen-induced complex formation and metal-to-non metal transition in an intermetallic compound. Such transitions are of both fundamental and technological interest as shown for binary systems such as Y-H [4]. In this article some recently investigated ternary and quaternary metal hydride systems having similar properties are reviewed.

## $Mg_3Ir-H$ system

Binary  $Mg_3Ir$  crystallizes with a hexagonal  $Cu_3P$ -type structure and is metallic. Hydrogenation yields a red colored, presumably non-metallic ternary hydride having a monoclinic distorted metal atom arrangement and the unusual composition  $Mg_6Ir_2H_{11}$  [5]. As can be seen in Fig. 1 its hydrogen substructure can be rationalized in terms of four symmetry independent hydride complexes, one square-pyramidal  $[IrH_5]^{4-}$  and three saddle-like  $[IrH_4]^{5-}$  of which two are disordered.



Each complex is surrounded by eight  $Mg^{2+}$  cations in a deformed cubic configuration and conforms to the 18-electron rule. The structure also contains five hydride anions,  $H^-$ , bonded to magnesium in tetrahedral and triangular configurations. The metal-hydrogen bond lengths within the complexes correspond to the sum of covalent radii and those involving the  $H^-$  anions to the sum of ionic radii (for values see Fig. 1). The shortest H-H contacts are of the order of

**Fig. 1:** Hydride complexes and hydride anions in monoclinic  $Mg_6Ir_2H_{11}$ ; the square-pyramidal  $[IrH_5]^{4-}$  complex and one out of three saddle-like  $[IrH_4]^{5-}$  complexes are ordered (100% H occupancy); only one out of four tetrahedral coordinated  $H^-$  anions is shown; metal-hydrogen distances (Å) refer to deuteride; adapted from [5].

$\sim 2.0$  Å and thus consistent with repulsive H-H interactions. These structural features suggest the limiting ionic formula  $4\text{Mg}_6\text{Ir}_2\text{H}_{11} = 5\text{MgH}_2 \cdot 19\text{Mg}^{2+} \cdot 2[\text{IrH}_5]^{4-} \cdot 6[\text{IrH}_4]^{5-}$  and the classification of the compound as a „complex“ rather than as an „interstitial“ hydride. Moreover, its colored appearance suggests the occurrence of a hydrogen induced metal-to-nonmetal transition similar to that in the  $\text{Mg}_2\text{Ni-H}$  system. Similar to the latter the transition in the  $\text{Mg}_3\text{Ir-H}$  system is reversible and involves Mg atom shifts of up to  $\sim 2$  Å. The structure analysis of the hydride required the combined use of neutron and synchrotron data and the modeling of anisotropic diffraction line broadening. The latter presumably occurred as a result of micro-twinning due to a temperature induced order-disorder phase transition similar to that in  $\text{Mg}_2\text{NiH}_4$ . With a total of 126 positional atom parameters the structure of  $\text{Mg}_6\text{Ir}_2\text{H}_{11}$  is the most complicated so far solved by powder diffraction methods among metal hydrides (for a summary of properties and a comparison with other hydrides see Table 1). A question that remains open is whether the formation of the metal-hydrogen complexes coincides with, or precedes the metal-to-nonmetal transition.

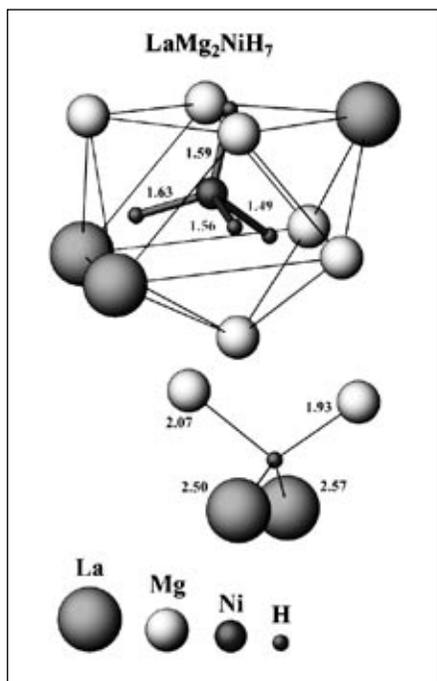
**Table 1:** Hydrogen induced complex formation and electron localization in intermetallic compounds.

compound (structure type) symmetry (space group)	hydride symmetry (space group, positional parameters)	complexes and H <sup>-</sup> anions	hydride properties	hydride formation*	ref.
$\text{Mg}_2\text{Ni}$ ( $\text{Mg}_2\text{Ni}$ -type) hexagonal ( $P6_322$ )	$\text{Mg}_2\text{NiH}_4$ monoclinic ( $C2/c$ , 20)	$[\text{NiH}_4]^{4-}$	non-metallic brownish	$\sim 300^\circ\text{C}$ $\sim 1$ bar	[2]
$\text{Mg}_3\text{Ir}$ ( $\text{Cu}_3\text{P}$ -type) hexagonal ( $P6_3cm$ )	$\text{Mg}_6\text{Ir}_2\text{H}_{11}$ monoclinic ( $P2_1/c$ , 126)	$3[\text{IrH}_4]^{5-}$ $[\text{IrH}_5]^{4-}5\text{H}^-$	non-metallic red	$\sim 400^\circ\text{C}$ $\sim 50$ bar	[5]
$\text{LaMg}_2\text{Ni}$ ( $\text{MgAl}_2\text{Cu}$ -type) orthorhombic ( $Cmcm$ )	$\text{LaMg}_2\text{NiH}_7$ monoclinic ( $P2_1/c$ , 70)	$[\text{NiH}_4]^{4-}$ $3\text{H}^-$	metallic dark grey	$< 200^\circ\text{C}$ $< 8$ bar	[6]
$\text{NdNi}_4\text{Mg}$ ( $\text{MgCu}_4\text{Sn}$ -type) cubic ( $F-43m$ )	$\text{NdNi}_4\text{MgH}_4$ orthorh. ( $Pnm2_1$ , 17)	$[\text{Ni}_4\text{H}_4]^{5-}$	metallic dark grey	$\sim 50^\circ\text{C}$ $\sim 7-8$ bar	[7]

\* all hydrogenation reactions are reversible

## LaMg<sub>2</sub>Ni – H system

Ternary LaMg<sub>2</sub>Ni is a new compound that crystallizes with an orthorhombic MgAl<sub>2</sub>Cu-type structure (ordered Re<sub>3</sub>B-type derivative). Recent work shows [6] that it yields a quaternary metal hydride of composition LaMg<sub>2</sub>NiH<sub>7</sub> that is presumably metallic (Table 1). It displays a nearly unchanged monoclinic metal atom substructure (atom shifts  $< 1$  Å) and an ordered hydrogen atom distribution. As can be seen in Fig. 2 the latter can be rationalized in terms of tetrahedral  $[\text{NiH}_4]^{4-}$  complexes and hydride anions H<sup>-</sup> surrounded by lanthanum and magnesium in tetrahedral configurations.



**Fig. 2:** Hydride complexes and hydrido anions in monoclinic  $\text{LaMg}_2\text{NiH}_7$ ; only one of two tetrahedral  $[\text{NiH}_4]^{4-}$  complexes and one out of six tetrahedral coordinated  $\text{H}^-$  anions are shown; metal-hydrogen distances ( $\text{\AA}$ ) refer to the deuteride; adapted from [6].

Magnesium and lanthanum appear as electron donors in agreement with the limiting ionic formula  $\text{La}^{3+}\text{Mg}^{+2}_2 \cdot [\text{NiH}_4]^{4-} 3\text{H}^-$ . The Ni-H distances compare well with those in other known 18-electron  $[\text{NiH}_4]^{4-}$  complexes such as in  $\text{Mg}_2\text{NiH}_4$  (1.54-1.57  $\text{\AA}$ ), while the Mg-H and La-H distances are consistent with those in the corresponding binary hydrides. These features suggest that the compound should be considered as a link between „interstitial“ and „complex“ metal hydrides. High-resolution synchrotron diffraction data were essential for structure determination and

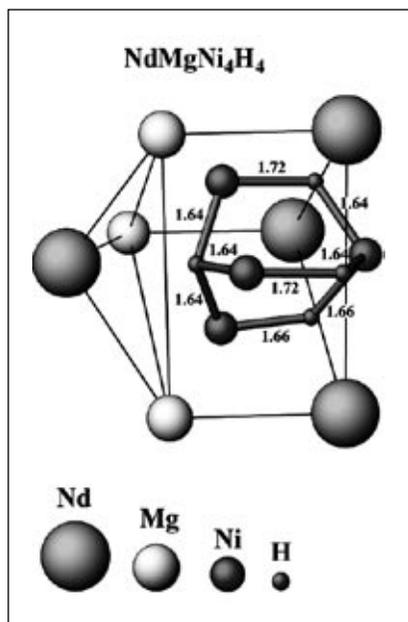
refinement because the monoclinic lattice distortion was initially not detected in the neutron and laboratory X-ray data and prevented the structure from being refined. An aspect that needs to be further investigated is the influence of metal-hydrogen complex formation on the electronic properties of the  $\text{LaMg}_2\text{Ni-H}$  system.

## **NdMgNi<sub>4</sub> – H system**

The ternary compound  $\text{NdMgNi}_4$  crystallizes with a cubic  $\text{MgCu}_4\text{Sn}$ -type structure (ordered  $\text{AuBe}_5$ -type derivative). As shown by recent work [7] it yields a quaternary metal hydride of composition  $\text{NdMgNi}_4\text{H}_4$  that has a nearly ordered hydrogen substructure and is presumably metallic (Table 1). The hydride forms at 7 bar and 50°C, is stable at room temperature and 1 bar hydrogen pressure, but loses hydrogen rapidly at 80°C under vacuum and decomposes under air by catalytic water formation. During hydrogenation the metal substructure remains nearly unchanged (atom shifts < 1  $\text{\AA}$ ) but undergoes an orthorhombic distortion while hydrogen fills trigonal bi-pyramidal  $[\text{Nd}_2\text{MgNi}_2]$  and tetrahedral  $[\text{NdNi}_3]$  type interstices. As shown in Fig. 3 the hydrogen substructure can be described in terms of a nearly ordered configuration of H ligands bridging three edges and one face of a nickel tetrahedron that is surrounded by four close lanthanum and three more distant magnesium cations.

**Fig. 3:** Hydride complex in orthorhombic  $\text{NdMgNi}_4\text{H}_4$ ; metal-hydrogen distances (Å) in  $[\text{Ni}_4\text{H}_4]^{5-}$  refer to the deuteride; adapted from [7].

The resulting  $[\text{Ni}_4\text{H}_4]^{5-}$  moiety is reminiscent of anionic hydride complexes and suggests that the compound is a further link between „interstitial“ and „complex“ metal hydrides. The Ni-H distances are consistent with covalent interactions while the La-H distances (2.34–2.50 Å) do not much differ from those in the ionic hydride  $\text{LaH}_3$  (~2.42 Å). A question that remains open is how the hydrogen substructure and electronic properties evolve at higher hydrogen contents (pressures).



## Conclusions and outlook

The above examples demonstrate that preferred hydrogen configurations similar to those in complex metal hydrides also occur in typically metallic („interstitial“) hydrides. Hydride formation is accompanied by a symmetry reduction and reversible changes in the metal substructure (atomic shifts of up to 2 Å, up to 126 positional parameters). Some hydrides are colored and display hydrogen-induced transitions from delocalized (alloy) to localized (hydride) electron states. The structures and compositions can be rationalized by electron counting rules suggesting that the compounds are links between „interstitial“ and „complex“ metal hydrides. Clearly, similar discoveries in other systems would confirm this view and open the door for a better understanding of metal-hydrogen interactions in metallic systems. High-resolution in-situ neutron diffraction experiments are in progress.

*Acknowledgements:* This review covers work performed by my collaborators whose names appear in the list of references. Particular thanks are due to G. Renaudin for help with the drawings. The work was supported by the Swiss National Science Foundation and the Swiss Federal Office of Energy.

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## Joël Mesot,

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### Winner of the ETHZ LATSIS Prize 2002

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A. Furrer, Laboratory for Neutron Scattering PSI & ETHZ



It is a great pleasure to announce that Joël Mesot, member of the Swiss Society for Neutron Scattering, received the ETHZ LATSIS Prize 2002, the most prestigious award for young scientists (less than 40 years old) in Switzerland. A special ceremony in honour of the laureate took place on 19 November 2002 at the University of Geneva, and the award was delivered at the ETHZ day on 23 November 2002.

Joël Mesot graduated from the ETHZ in the year 1992 with a Ph.D. thesis mainly performed at the ILL Grenoble. Afterwards he worked as an instrument scientist at the Laboratory for Neutron Scattering (LNS ETHZ & PSI). From 1997-1999 he spent two years at

the Argonne National Laboratory (ANL) through a grant by the Swiss National Science Foundation. Since October 1999 he is back at the LNS where he is presently the leader of the neutron spectroscopy group.

Joël Mesot's scientific career started in an exciting period for physicists, namely some years after the discovery of high-temperature superconductivity (Bednorz & Müller, Nobel prize in physics, 1987). Joël Mesot's early works concerned the static and dynamic magnetic properties of high-temperature superconductors studied by neutron scattering techniques. For this purpose he designed and realised (in co-operation with a group from the University of Saarbrücken) the novel spectrometer FOCUS at SINQ which allows highly resolved neutron spectroscopy experiments. His neutron scattering studies showed that the high- $T_c$  superconductors are intrinsically inhomogeneous, i.e., the superconductivity occurs through a percolation process. For this work he received several prizes, e.g., the IBM prize 1995 of the Swiss Physical Society.

During his stay at ANL Joël Mesot got acquainted with photoemission techniques at synchrotron sources in order to study the electronic properties of high- $T_c$  superconductors. He became an internationally acknowledged expert in angle-resolved photoemis-

sion spectroscopy (ARPES) experiments which allow a very direct determination of the nature and size of the superconducting gap. In particular, together with his collaborators he could show that the electronic and magnetic degrees of freedom are strongly coupled which is an important result towards the understanding of high- $T_c$  superconductivity.

Back at the LNS Joël Mesot and his collaborators achieved further important results. For the first time the flux-line lattice of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  could be established by small-angle neutron scattering. The field dependence of the flux-line lattice is highly intriguing; while it is hexagonal at low magnetic fields, it transforms into a quadratic structure at higher fields. This result which was highlighted on the front page of the Physical Review Letters (27 May 2002, Volume 88, Number 21) is a further important step to narrow down the possible mechanisms for the yet unsolved phenomenon of high- $T_c$  superconductivity.

We all congratulate Joël Mesot for his outstanding achievements and wish him a successful continuation of his scientific career.

# *Photo-Crystallography at TriCS/SINQ:*

## *Light-induced structural changes in*

### *$\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{H}_2\text{O}$*

*D. Schaniel, J. Schefer, Laboratory for Neutron Scattering, ETHZ & PSI  
T. Woike, Institut für Mineralogie und Geochemie, Universität zu Köln  
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## **Introduction**

The light-induced metastable electronic states in single crystals of nitrosyl-compounds like  $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{H}_2\text{O}$  (Sodiumnitroprusside, SNP) are of fundamental interest because of their extremely long lifetime of  $\tau > 10^8\text{s}$  below characteristic decay temperatures and the reversibility of the excitation process [1]. They can be used for optical information storage with very high capacity by volume holography (see Fig. 1 for illustration). The modulation of the refractive index is  $\Delta n \geq 4 \cdot 10^{-2}$ , which exceeds those of the well known photorefractive materials like doped  $\text{LiNbO}_3$ ,  $\text{BaTiO}_3$ ,  $\text{LiTaO}_3$ ,  $\text{Sr}_x\text{Ba}_{1-x}\text{Nb}_2\text{O}_6$ , etc. by at least two orders of magnitude.

In SNP two metastable states SI and SII can be excited by irradiation with light below the characteristic decay temperatures of 198 K and 147 K, respectively. About 50% of the

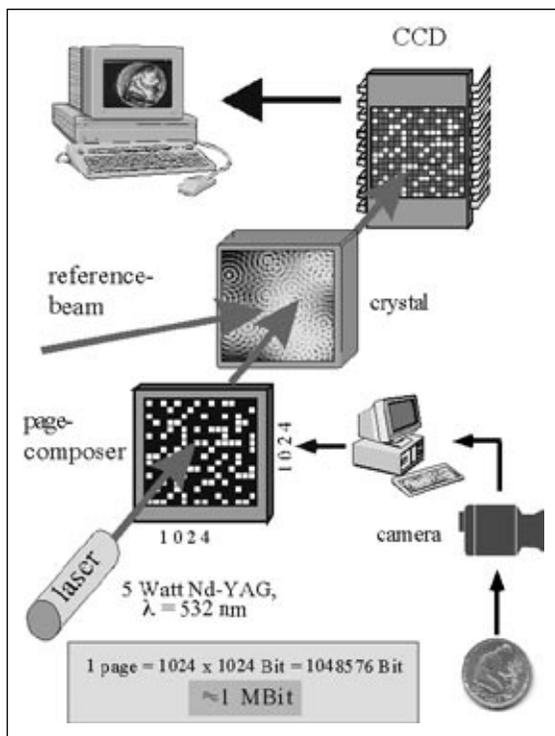
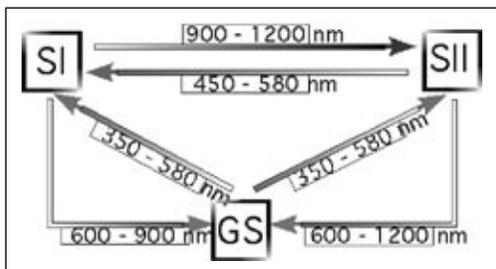


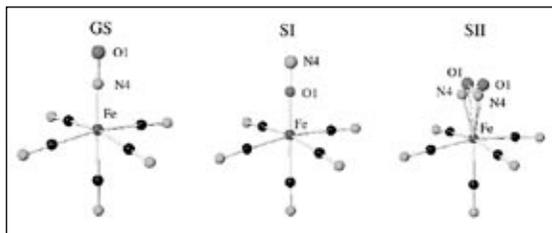
Figure 1: Typical setup for writing and reading of holographic information, using a single crystal.

$[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ -molecules can be transferred into SI with a light polarization perpendicular to the quasi four-fold axis N-C-Fe-N-O using a wavelength of 440-470 nm. Relaxation into the ground state (GS) takes place by irradiation with light in the spectral range of 600-1200 nm or by thermal heating over the decay temperatures, whereby illumination with light in the region of 900-1200 nm transfers about 32% of the anions in SII and the rest into the ground state (see Fig. 2).

**Figure 2:** Schematic view of the excitation processes in SNP.



The new states SI, SII are located energetically about 1 eV above the ground state [2]. From the structural point of view there are two different results: Based on neutron diffraction experiments it was proposed that only the Fe-N and N-O bond distances are elongated by a small amount [3,4] whereas X-ray diffraction results can be explained also by an isonitrosyl configuration (inversion of the nitrosyl ligand from Fe-NO to Fe-ON) for SI and a *side-on* ( $\eta^2$ ) configuration of the nitrosyl ligand for SII [5]. Thus the reaction coordinates Q for the two excitations are either the rotation angle  $\varphi_{\text{SI}}=180^\circ$  for the isonitrosyl configuration (SI) or the rotation angle  $\varphi_{\text{SII}}=90^\circ$  for the *side-on* configuration in SII (see Fig. 3). Density Functional Theory (DFT) calculations showed, that the isonitrosyl and *side-on* configurations are indeed stable energetic minima [6]. For SI the quasi  $C_{4v}$  ( $4m$ ) symmetry of the  $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ -molecules is conserved, whereas for SII it is reduced to  $C_s$  ( $m$ ), thereby lifting all degeneracies of vibrational bands and electronic orbitals, as detected by polarized absorption spectroscopy [7]. However, no splitting of the e-modes in SII could be detected by Raman or Infrared spectroscopy [8,9,10,11]. The space group Pnnm is unchanged, no new reflections could be detected, so that in the  $90^\circ$ -configuration of SII the N-O ligands are perpendicular to each other (see Fig.3), in order to conserve the mirror plane m.

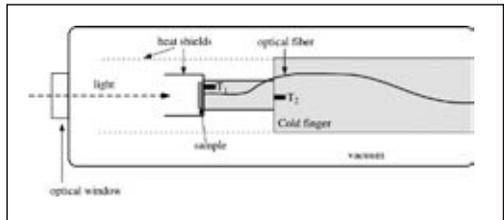


**Figure 3:** Ground state, isonitrosyl (SI) and side-on (SII) configuration of SNP as proposed by Carducci et al.[5]

## Photo-Crystallographic Experimental Set-Up

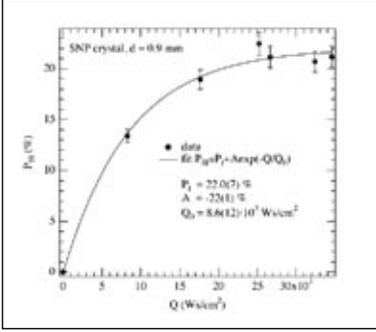
The neutron diffraction experiments were performed on the single-crystal diffractometer TriCS at the Swiss Spallation Source SINQ at PSI/Villigen using a single detector. The SNP samples were mounted on a sample holder as indicated in Figs. 4,5 in a closed cycle refrigerator (CCR). The refrigerator is equipped with an optical window (quartz) to allow for the illumination of the sample with polarized light down to temperatures of 15 K. In order to guarantee thermal stability at low temperature additional heat shields (aluminum) were mounted. The temperature was measured with two sensors: one is placed directly behind the sample position ( $T_1$  in Fig. 4) and a second one ( $T_2$ ) is mounted on the cold finger of the CCR. A deuterated single crystal of SNP (diameter 9 mm, thickness 0.9 mm) was used. First, the mixed state GS+SI was excited by illuminating the crystal with laser light of wavelength 476.5 nm and with polarization along the  $c$ -axis of the crystal. The average intensity was  $100 \text{ mW/cm}^2$  so that after 100 h of illumination time a total exposure  $Q \approx 36000 \text{ Ws/cm}^2$  was achieved. After the measurement of a full data set at 43 K (sensor  $T_1$ ) of the excited state (1134 reflections) the crystal was heated to 200 K in order to depopulate SI. Afterwards the same data set was measured in the GS at 43 K (sensor  $T_1$ ).

**Figure 4:** Schematic drawing of the photo-crystallographic setup used in the TriCS experiment.



The population of the metastable states during the neutron scattering experiment can be determined by measuring the transmitted light intensity behind the SNP crystal. The light intensity can be measured with a Si-photo diode. The voltage over the diode is proportional to the transmitted light intensity. An amplifier with selectable load resistors guarantees a linear behaviour over many decades. A fiber optic was introduced in the refrigerator guiding the light to the photo diode, which is working stable at room temperature. Fig. 5 shows the population measured on a SNP

**Figure 5a:** SNP crystal mounted in the refrigerator. The black cable on top is the optical fiber used for the transmission measurement.



**Figure 5b:** Population as a function of light exposure  $Q$ .

crystal of thickness  $d=0.9$  mm, which was illuminated at 43 K (sensor  $T_1$ ) with laser light of the wavelength 476.5 nm and an average power of  $100 \text{ mW/cm}^2$ . The measured voltage  $U_{ph}$  is proportional to the transmitted light intensity  $I_t$ , given by the incident light intensity  $I_0$  of the laser beam and the damping in the sample

$$U_{ph} \sim I_t = I_0 e^{-\alpha d} \quad (1)$$

where  $\alpha$  is the absorption coefficient of the sample and  $d$  is the thickness of the sample. Measuring the transmitted light intensity one can therefore determine the absorption coefficient of the crystal by

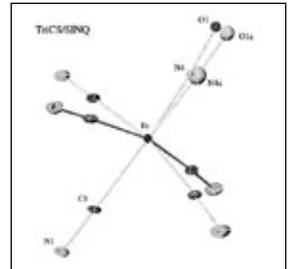
$$\alpha_{GS+SI}(Q) = \alpha_{GS}(Q=0) - \frac{1}{d} \ln \left( \frac{I_t, GS+SI}{I_t, GS} \right) \quad (2)$$

The absorption coefficients of GS and of the mixed states GS+SI are precisely known from optical absorption measurements [7]. Therefore the population of the metastable state SI can be determined by comparing  $\alpha_{GS+SI}(Q)$  and  $\alpha_{GS}(0)$  at the corresponding wavelength (476.5 nm) with the absorption curves.

## Results

The neutron diffraction data of the mixed state GS+SI (22% SI) can be refined by introducing two NO ligands: N4-O1 for GS and N4a-O1a for SI (see Fig.6). The displacement parameters for Fe, N4, N4a, O1, and O1a have to be chosen isotropic.

The main changes between GS and SI in this model occur at the C1-Fe-N4 bond. The Fe-N4 (GS) distance is increased from  $1.67(1) \text{ \AA}$  to  $1.72(2) \text{ \AA}$  in Fe-N4a (SI). The C1-Fe-N4 angle is almost  $180^\circ$  in SI (C1-Fe-N4a) whereas for GS it is about  $176^\circ$ . The N4-O1 (N4a-O1a) distance and the Fe-N4-O1 (Fe-N4a-O1a) angle remain practically unchanged. Fig. 6 illustrates the finding that



**Figure 6:** View of the  $Fe[(CN)_5NO]$ -molecule along the  $c$ -axis of the crystal ( $10^\circ$  inclined) in the model with two NO ligands. The two NO ligands of the GS (N4-O1) and SI (N4a-O1a) are indicated on the same molecule.

for SI the quasi-fourfold-axis of the molecule is nearly in a linear configuration, whereas for the GS it shows a slight bending away from the fourfold axis.

Introducing an isonitrosyl configuration for SI, i.e an inverted NO ligand O1a-N4a beside the GS configuration, no stable refinement with physically meaningful parameters can be obtained, e.g. the displacement parameters are negative.

## Conclusions

The neutron diffraction experiments on the metastable excited state SI of SNP do not support the model proposing an isonitrosyl configuration of the nitrosyl ion (Fig. 3). Instead the structural refinement of the neutron data shows that a small but significant change in the Fe-N bond length ( $\sim 0.05 \text{ \AA}$ ) and in the C-Fe-N angle ( $\sim 3.5^\circ$ ) are the only rearrangements in the structure connected with the excitation of the metastable state SI [12,13]. The x-ray experiments can be explained equally well with both models (isonitrosyl and small change in Fe-N bond length) as stated by the authors of the x-ray study [5]. However, such a small structural change after the irradiation can not explain the extremely long life time [14]. A significant redistribution of the charge density must be connected with the excitation of SI, which may also explain why the analysis of x-ray diffraction data does not yield unambiguous results.

An entire photo-crystallographic setup was built at TriCS/SINQ to detect light-induced structural changes by irradiation with light in the blue-green spectral range at temperatures between 15 K and 300 K. An extension to other spectral ranges is possible with the corresponding lasers.

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# *AMOR – the multi-option time-of-flight reflectometer at SINQ/PSI*

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## **Introduction**

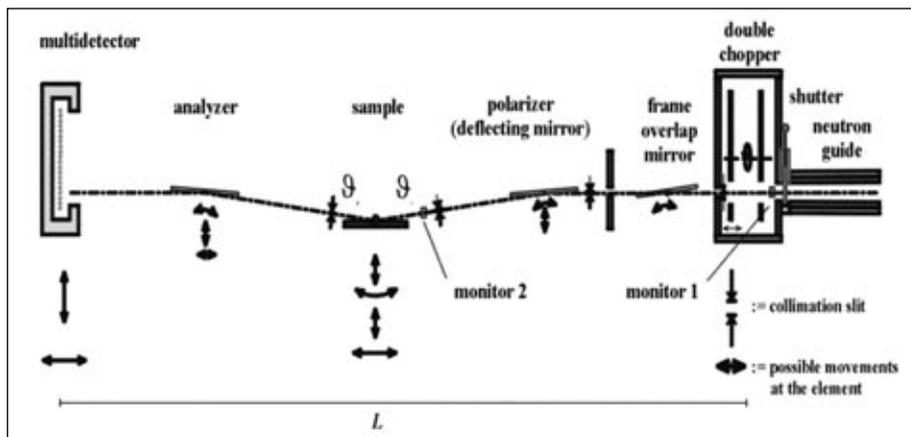
In recent years x-ray and neutron reflectometry have been established as nondestructive microscopic probes for the investigation of stratified structures and hidden interfaces. Due to the unique interaction of neutrons with matter, specular neutron reflection probes the atomic and magnetic scattering length densities perpendicular to the sample surface. It can be very sensitive to electrochemical processes at interfaces as well as to surface and interface magnetism. Moreover polymer interfaces and biological model membrane systems can be studied using contrast variation. Growth, wetting, adsorption and adhesion, inter-diffusion, surface magnetism, magnetic excitations, thin film superconductivity, dynamics at interfaces all are research fields applicable to neutron reflectometry.

An extremely flexible state of the art time-of-flight reflectometer becomes now available at the swiss neutron source SINQ at PSI. AMOR – the apparatus for multi-option reflectometry at SINQ/PSI is adaptable to the experimental demands of surface and interface studies in the various fields of research [1,2].

## **Basic instrument concept**

The principal setup of AMOR allows measurements with polarized or unpolarized neutrons in white beam time-of-flight mode ( $1.3 \text{ \AA} < \lambda < 13 \text{ \AA}$ ) and optionally in unpolarized monochromatic  $\theta$ - $2\theta$  mode. The latter mode is implemented with a thin film Ni/Ti multilayer monochromator consisting of 1500 layers and a d-spacing of 5 nm.

The scattering plane of the sample is oriented vertically in order to allow measurements at open liquid surfaces, too. The inclination angle and thereby the accessible q-range is adjusted by tilting a deflection mirror and/or the sample. A flexible software control of the  $\theta$ - $2\theta$ -movement around axes that are not mechanically coupled has been implemented. The standard mode of the instrument is time-of-flight, which has been opened for user operation in Oct. 2002. An area detector or two single detector tubes can be operated alternatively with new fast detector read-out electronics.



*Fig. 1: Reflectometer AMOR at SINQ/PSI and principal layout.*

Most optical components are riding on an 8m optical bench so that the chopper-detector distance can be varied in order to give an optimum sample illumination and resolution (Fig. 1).

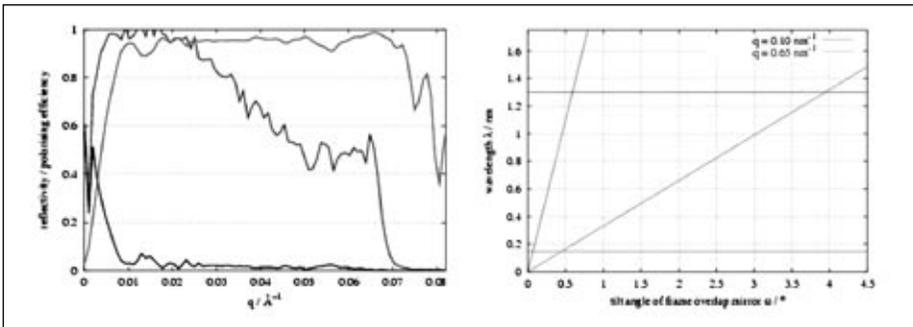
## Layout of instrument components

### Chopper system

A cold neutron beam from the end position of the curved neutron guide ( $m = 2$ ) 1RNR17 with a flux of  $1.38 \times 10^8 \text{ n cm}^{-2} \text{ s}^{-1} \text{ m A}^{-1}$  (averaged over the spectrum) hits a double chopper system defining the origin of the neutron burst of the instrument. The neutron guide has a cross section of  $5 \times 5 \text{ cm}^2$ . The spectral distribution obtained from the liquid  $\text{D}_2$  moderator at SINQ offers a wide usable wavelength band which peaks at  $\lambda_{\text{max}} = 0.4 \text{ nm}$ . The two chopper discs have two slits at  $180 \text{ deg}$ . They are phase coupled with a max. speed of  $6000 \text{ rpm}$  giving burst rates of  $200 \text{ Hz}$ . The distance chopper-detector is variable between  $3.5 - 10 \text{ m}$ . The chopper frequency, width of the gating window and the chopper-detector distance can be defined independently. Hence the resolution can be optimally tuned to the experimental needs.

## Optics

A frame overlap mirror consisting of a Si based Ni/Ti supermirror ( $m=2$ ) positioned behind the chopper system eliminates undesired neutrons with wavelengths larger than 1.3 nm. Following to this position is a station that can be equipped by either a deflecting mirror of a highly oriented pyrolytic graphite (HOPG) double monochromator to give a monochromatic beam of  $\lambda = 0.4735$  nm or by a remanent polarizing FeCoV/Ti: N supermirror that can operate for a broad wavelength band of polarized neutrons. The performance of the polarizing mirror is shown in Fig. 2.



**Fig. 2:** Reflectivity and resulting polarization of polarizer/analyzer supermirror installed at AMOR (left). Available wavelength band (right).

The sample stage to align the sample horizontally (vertical scattering geometry) is equipped with two rotation angles and a translation in  $z$ . Samples of size of up to  $150 \times 500 \text{ mm}^2$  can be measured at ambient atmosphere when placed on a standard sample mount.

Behind the sample stage a reflecting mirror analogue to the deflecting polarizing mirror can be installed for the polarisation analysis of the reflected beam. Between frame overlap mirror and sample and sample and detector various diaphragms can be placed in order to define the beam. To fulfil the requirements of experimental stability and vibration control all devices are installed on a 8 m long solid optical bench, where they can be moved along the beam direction (see Fig. 1).

## Detectors

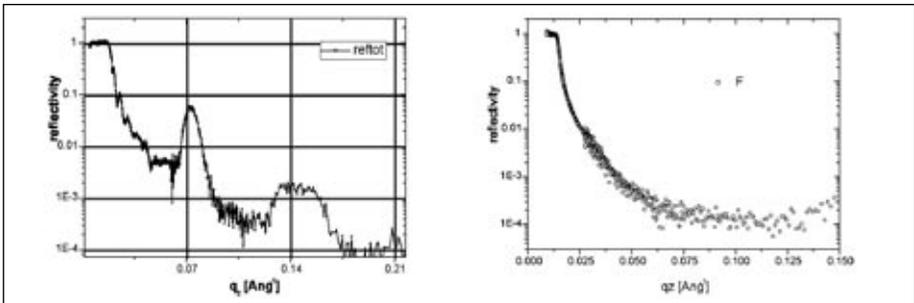
Two  $^3\text{He}$  single detector tubes and one  $^3\text{He}$  two dimensional multiwire position sensitive detector (PSD) are installed on AMOR. The EMBL 2D-PSD has an active area of  $172 \times 190 \text{ mm}^2$  with less than 2 mm spatial resolution. Obtained monochromatic and time-of-flight data are stored in HDF5/NEXUS file format.

## Sample environment

The flexibility of the instrument also allows for large sample environments, such as cryomagnets, evaporation chambers, furnaces or Langmuir troughs. Currently a 1.5 T electromagnet with a horizontal field operational at room temperature, two Helmholtz coils for a small horizontal field up to 150 G applicable around larger sample stages, a 11 T cryomagnet with a horizontal field and a temperature range between 1.5 – 300 K, and a Langmuir trough for measurements at the air-liquid interphase, are provided as special sample environments on AMOR. A sample cell for measurements at the solid-liquid interface and a dedicated furnace to be used in reflectivity measurements will be developed soon.

## Conclusions

The neutron reflectometer AMOR offers extremely flexible opportunities to measure all kinds of multilayered structures, magnetic or non-magnetic, to study phenomena at solid-solid or solid-liquid interfaces (adsorption, wetting and de-wetting, diffusion etc.) and, due to the horizontal sample geometry, phenomena at air-liquid and liquid-liquid interfaces. Recent examples of the measurement of a Fe/Cr multilayer system at AMOR in time-of-flight mode and of a D<sub>2</sub>O air-liquid surface are shown in Fig. 3.



**Fig. 3:** Reflectivity of a Fe/Cr multilayer (left) and liquid D<sub>2</sub>O (right) measured in tof-mode at AMOR.

## References

- [1] D. Clemens, Physica B, **221**, 507 (1996)
- [2] D. Clemens et al., Physica B, **276-278**, 140 (2000)

# *Announcements*

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## **New SGN/SSDN Members**

The Swiss Neutron Scattering Society welcomes the following new members:

- P. Strunz (LNS, PSI&ETHZ)
- S. Valloppilly (TU Munich)
- J. Loverio (University of Singapore)
- A. Sieber (University of Bern)
- S. Ochsenbein (University of Bern)
- T. Gutberlet (LNS, PSI&ETHZ)

Presently the SGN has 189 members.

## **SINQ User Program**

For the recent deadline (15/11/02) the SINQ scientific coordination office received 89 proposals for the 10 instruments in user operation, as many as never before. 66 out of those are shortterm proposals. The share of new proposers who never did an experiment at SINQ before is 41%. At the end of January 2003 after the next SINQ committee meeting the proposers will be informed about the acceptance/rejection of their proposals.

## **SINQ Proposal Deadline**

The next deadline for the submission of proposals for SINQ will be

15 May 2003

For more detailed information please have a look at the SINQ webpages: ([sinq.web.psi.ch](http://sinq.web.psi.ch)).

## Conferences 2003

date	place	conference
08–09/01	Villigen	PSI $\mu$ SR Users' Meeting
16/01	Villigen	5 <sup>th</sup> SINQ Users' Meeting
16–21/01	San Diego	4 <sup>th</sup> Intern. Conference on Superconductors and Related Materials <a href="http://www.phys.subr.edu/conference/new3sc.htm">www.phys.subr.edu/conference/new3sc.htm</a>
22–25/01	Grenoble	2nd Workshop on Dynamics in Confinement <a href="http://www.ill.fr/Events/Onsite/confit2003/confit.html">www.ill.fr/Events/Onsite/confit2003/confit.html</a>
17–21/02	Berlin	24 <sup>th</sup> HMI Tutorial Session on Neutr. Scatt.
03–07/03	Austin	APS March Meeting <a href="http://www.aps.org/meet/MAR03">www.aps.org/meet/MAR03</a>
20–21/03	Basel	Annual Meeting of the Swiss Phys. Society <a href="http://www.sps.ch">www.sps.ch</a>
24–28/03	Dresden	Spring Meeting 'Solid State Physics' of the German Physical Society <a href="http://www.dpg-tagungen.de/info/hannover2003.html">www.dpg-tagungen.de/info/hannover2003.html</a>
08–10/05	Poznan	10 <sup>th</sup> Int. Seminar on Neutron Scattering in Condensed Matter <a href="mailto:nawrocik@main.amu.edu.pl">nawrocik@main.amu.edu.pl</a>
12–15/05	Neuss	ICANS XVI <a href="mailto:j.philippen@fz-juelich.de">j.philippen@fz-juelich.de</a>
19–30/05	Trieste	Spring School on "Magnetic Properties of Condensed Matter Investigated by Neutron Scattering and Synchrotron Radiation" <a href="mailto:moze@mail.unimo.it">moze@mail.unimo.it</a>
25–30/05	Rio de Janeiro	7 <sup>th</sup> Int. Conference on Materials and Mechanisms of HTSC <a href="http://www.m2srio.cbpf.br">www.m2srio.cbpf.br</a>

<b>date</b>	<b>place</b>	<b>conference</b>
08-11/06	Dubna	XII <sup>th</sup> Int. Conf. On Selected Problems of Modern Physics <a href="http://www.thsun1.jinr.ru/~pqft/">www.thsun1.jinr.ru/~pqft/</a>
06-11/07	Linz	14 <sup>th</sup> Int. Conf. On Solid Compounds of Transition Elements Scte2003@jku.at
27/07–01/08	Rome	International Conference on Magnetism (ICM) <a href="http://www.icm2003.mlib.cnr.it">www.icm2003.mlib.cnr.it</a>
04–06/08	Venice	Int. Conf. on Polarised Neutrons and Sync. X-rays for Magnetism (PNSXM 2003) <a href="http://venice.infm.it/">http://venice.infm.it/</a>
24–29/08	Geneva	Int. Conference on f-Elements (ICFE '5) <a href="http://ereswww.epfl.ch">http://ereswww.epfl.ch</a>
03–06/09	Montpellier	3 <sup>rd</sup> European Conference on Neutron Scattering (ECNS 2003) <a href="http://www.ldv.univ-montp2.fr:7082/~ecns2003/">http://www.ldv.univ-montp2.fr:7082/~ecns2003/</a>
03–06/09	Szczecin	7 <sup>th</sup> Int. Conf. on Intermolecular and Magnetic Interactions nikos.guskos@ps.pl
14–19/09	Stara Lesna	Structure Solution from Powder Diffr. Data <a href="http://www.sspd-03.sav.sk/">http://www.sspd-03.sav.sk/</a>

# *The First American Conference on Neutron Scattering*

*Holger Kohlmann, Department of Physics, University of Nevada, Las Vegas*

A dream of many neutron scatterers in America finally came true, when the first American Conference on Neutron Scattering (ACNS, [www.sns.gov/acns](http://www.sns.gov/acns)) was organized by the Neutron Scattering Society of America (NSSA, [www.neutronscattering.org](http://www.neutronscattering.org)) in conjunction with the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) User Group (SHUG). 350 scientists from academia (47% from universities), research laboratories (43% from national neutron centers / US government laboratories) and industry (2%) from America and overseas (8%, participants from Brazil, England, France, Germany, Japan, Latvia, Netherlands, Poland, Russia, Spain, and Sweden) gathered in Knoxville, Tennessee, June 23–27, 2002, for this inaugural conference. Scientists from many different disciplines were brought together, such as biology, chemistry, engineering, materials science, metallurgy, physics, thus reflecting the interdisciplinary character of neutron scattering and of the NSSA. It is intended to hold ACNS every other year in years not coinciding with the International or the European Conference on Neutron Scattering.

After welcome words from the organizers and sponsors (NSSA, DOE, NSF, etc.) NSSA President Jim Rhyne announced the establishment of the NSSA Clifford G. Shull Prize in Neutron Science. Clifford Shull, who passed away on March 31, 2001, received the Nobel Prize in 1994 for the development of the neutron diffraction technique (along with Bertram Brockhouse, for the development of neutron spectroscopy). The NSSA Clifford G. Shull Prize in Neutron Science will be given to an individual making outstanding contributions to the field of neutron science, first to be awarded during ACNS 2004.

The scientific part of the conference started with reviews of neutron sources in the US (Paul Sokol, Penn State University) and in the world (Gerry Lander, European Institute of Transuranium Elements) and an SNS overview (Thom Mason, SNS). Naturally, the Spallation Neutron Source ([www.sns.gov](http://www.sns.gov)), currently under construction in Oak Ridge, Tennessee (see web cam at [it.sns.ornl.gov/webcam/](http://it.sns.ornl.gov/webcam/)), received major attention. SNS is a 1.4 G\$ project and will provide the USA's most powerful tool in neutron science, when completed in 2006. Conference participants had a chance to see the progress with their own eyes on a tour to the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS) construction site (Fig. 1). For more up-to-date information on SNS visit the website [www.sns.gov](http://www.sns.gov). It was also clearly pointed out that SNS

is only a first step to close the gap between neutron science in America and Europe. Other measures, such as improvements in the existing neutron facilities were suggested (see also the report “The Status and Needs of Major Neutron Scattering Facilities and Instruments in the United States“, available online at <http://www.ostp.gov/html/NeutronIWGReport.pdf>).



**Fig. 1:** SNS storage ring, target station (to be built) and LINAC, June 27, 2002. Compare with the current status of the SNS site ([web cam at it.sns.ornl.gov/webcam/](http://webcam.at.sns.ornl.gov/webcam/))!



A project similar to SNS as for size, budget and anticipated performance is the Japanese JAERI and KEK joint High Intensity Proton Accelerator Project ([jkj.tokai.jaeri.go.jp](http://jkj.tokai.jaeri.go.jp)), which will strengthen Japans position in neutron science in Asia.



Neutron science was discussed in plenary and keynote talks, sessions on specialized subjects, and poster sessions, and reflected the interdisciplinarity of the field. Topics ranged from Biomolecules and Polymers over Materials Chemistry, Hydrides and Magnetism to Neutron Techniques and

Nuclear, Particle and Astrophysics, to name just a few. Robert Cava (Princeton University) gave an excellent overview of current directions in materials research, some of which aim at characterization by neutron scattering. An example is the *in situ* investigation of hydrothermal synthesis of important materials, such as zeolites, as pointed out in a keynote lecture given by Dermot O’Hare (University of Oxford). Other interesting *in situ* neutron techniques were presented in several posters, and the application of *in situ* high pressure techniques was discussed by Chris Tulk (SNS) and Alexander I.

Kolesnikov (ANL). Ferenc Mezei (LANL and HMI) pointed out that by making use of supermirror neutron optics and / or repetition rate multiplication at a pulsed source the resolution of instruments can be increased by increasing the length of the instrument at no cost as for intensity. This finding is called “Free Lunch Theorem” and is of course of great importance for instrument design at new neutron sources such as SNS and also ESS. The recently discovered superconductivity in MgB<sub>2</sub> at 39K was discussed in a keynote lecture given by Jim Jorgensen (ANL), where he pointed out the importance of the chemistry of this simple compound, e. g. accidental doping by impurities in starting materials.



**Fig. 2:** Ian Anderson, Experimental Facilities Division Director of SNS, in his newly adapted “southern-like” outfit (after dinner speech at the banquet)

The location of the venue, Knoxville, Tennessee, was ideal for short visits in the surrounding areas, e. g. to the Great Smokey Mountain National Park (<http://www.nps.gov/grsm/gsmsite/home>) with its plentiful diversity of plants and wildlife. The perfect organization of the conference, the southern hospitality and social events such as the conference banquet (Fig. 2) contributed considerably to make ACNS 2002 an enjoyable experience. The next ACNS will be held in 2004 at a location yet to be determined.



# SINQ

Swiss Spallation Neutron Source

**RESEARCH PROPOSAL**

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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, $\Delta E$ , $\lambda$ , $\Delta\lambda$ , Q, $\Delta Q$

**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: \_\_\_\_\_