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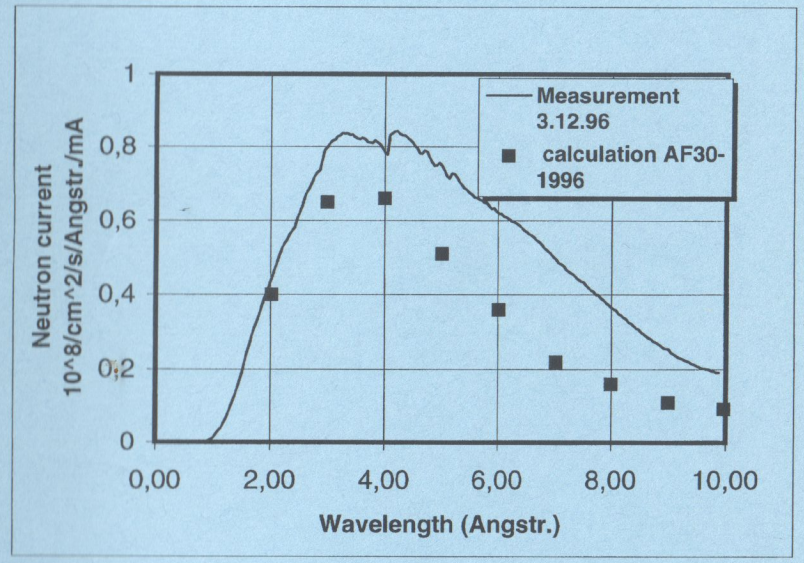
SWISS NEUTRON NEWS



Schweizerische Gesellschaft für Neutronenstreuung
Société Suisse pour la Diffusion des Neutrons
SGN / SSDN

Cover illustration:
First Neutrons from the Swiss Spallation Source at PSI: TOF-Spectrum measured on Dec. 3 1996 at SINQ-RNR14 guide with supermirror coating (m=2). See the report by W.Fischer in this issue.

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Inhaltsverzeichnis

Editorial

Während Synchrotronstrahlungsquellen überall fast "wie Pilze aus dem Boden spriessen" (ins Deutsche übersetztes Originalzitat von Stephen Lovesey), beginnt die Welt bezüglich Neutronenquellen langsam auszutrocknen ("the neutron drought"). Wie wohltuend war deshalb in diesem Umfeld die kürzlich erfolgte Inbetriebnahme der Spallationsneutronenquelle SINQ am PSI! Sie wird nicht nur uns Schweizern als nationale Basis für Ausbildung, Forschung und Anwendungen der Neutronenstreuung zur Verfügung stehen, sondern sie erfüllt auch eine wichtige Funktion im europäischen Netzwerk der Neutronenquellen.

Stillstand heisst Rückschritt! Trotz der SINQ dürfen wir uns nicht behaglich zurücklehnen; wir müssen jetzt den ersten Schritt in die Zukunft tun, wollen wir die führende Stellung Europas auf dem Gebiet der Neutronenstreuung erhalten und weiter ausbauen. Und dieser Schritt heisst **European Spallation Source (ESS)**. Vor kurzem ist eine dreibändige Projektstudie der ESS publiziert worden; alle Mitglieder unserer Gesellschaft werden diese Unterlagen in den nächsten Wochen erhalten. Jetzt folgt eine intensive R&D Phase, an der sich auch das PSI beteiligt. Die Planung sieht vor, dass die ESS im Jahre 2010 in Betrieb gehen wird mit einem anvisierten Neutronenfluss, der vierzigmal höher ist als bei der heute weltbesten Spallationsquelle ISIS! Damit kann man Forschungsprojekte angehen, die heute - trotz ständigen Fortschritten in der Instrumentierung - noch nicht möglich sind. Insbesondere wird man in der Lage sein,

- in Raum und Zeit höchstaufgelöste Experimente durchzuführen,
- von der Polarisationsanalyse vollen Gebrauch zu machen,
- "real time" Phänomene in kurzen Zeitskalen zu studieren,
- auch kleinste Probenmengen und Oberflächen zu untersuchen,
- extremste Bedingungen der Probenumgebung zu realisieren.

Die European Science Foundation (ESF) wird das Projekt ESS evaluieren. Es kann nur dann realisiert werden, wenn die europäische Nutzergemeinschaft volle Unterstützung gibt. Auch die Schweizerische Gesellschaft für Neutronenstreuung ist zu einer Stellungnahme aufgerufen, die wir an der kommenden Generalversammlung vom 21. November 1997 verabschieden werden. Ich rufe deshalb alle unsere Mitglieder auf, sich aktiv an dieser Meinungsbildung zu beteiligen. Wir haben die Gelegenheit, an der Grundsteinlegung für das "Neutronenhaus Europa" des kommenden Jahrtausends mitzuwirken. Nutzen wir diese Chance!

Albert Furrer
Präsident der SGN

Villigen, Juni 1997

First Neutrons from the Swiss Spallation Neutron Source at PSI

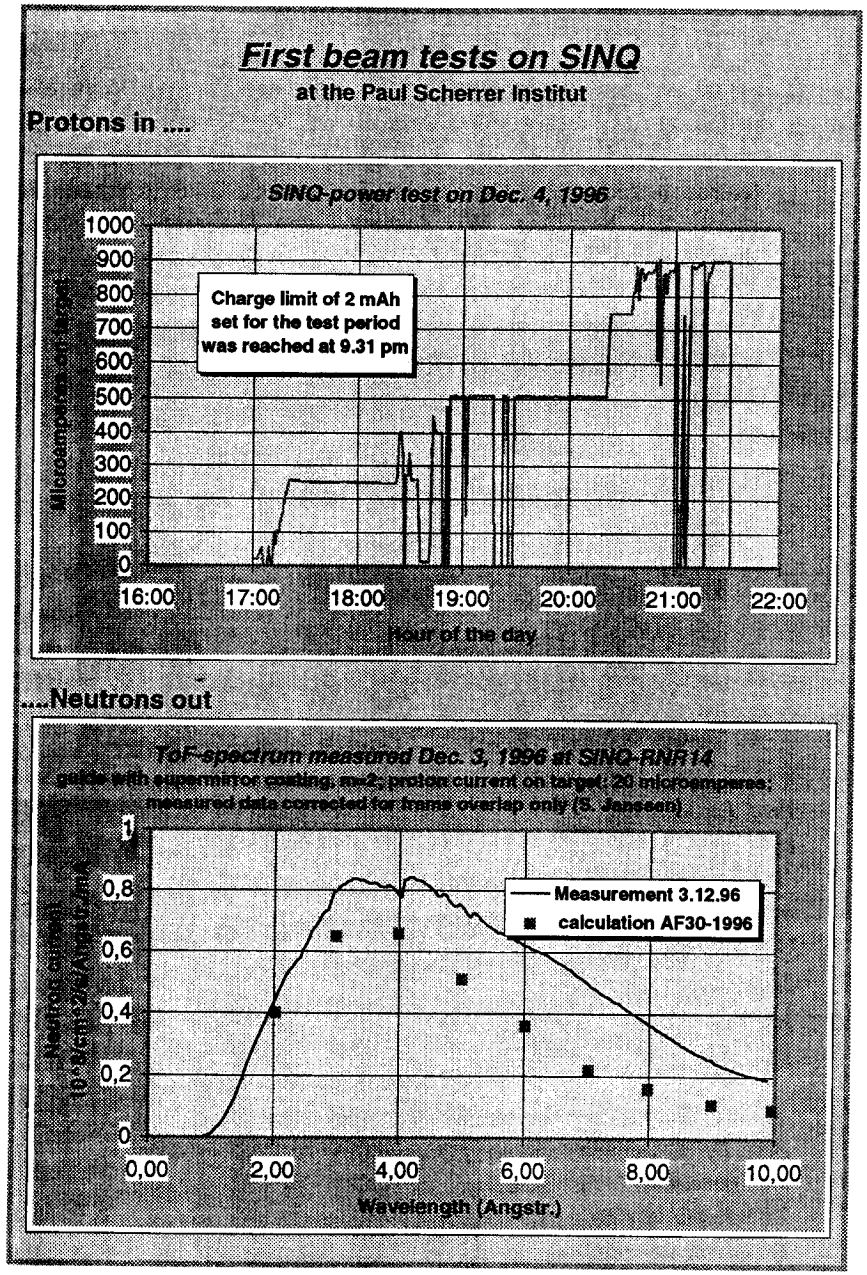
W.E. Fischer, Paul Scherrer Institut

On December 3, 1996 the Swiss Spallation Neutron Source (SINQ) was, for the first time, fed by the proton beam. The beam current for this first test of the neutronics performance was 20 μA. Flux measurements at the supermirror guide system have been carried out. Furthermore the spectral distribution from the cold source was measured.

The performance of the source with the installed "day-one" target was somewhat above our latest expectations. With the lead target, planned to be installed as soon as possible the neutron flux values will be twice as high.

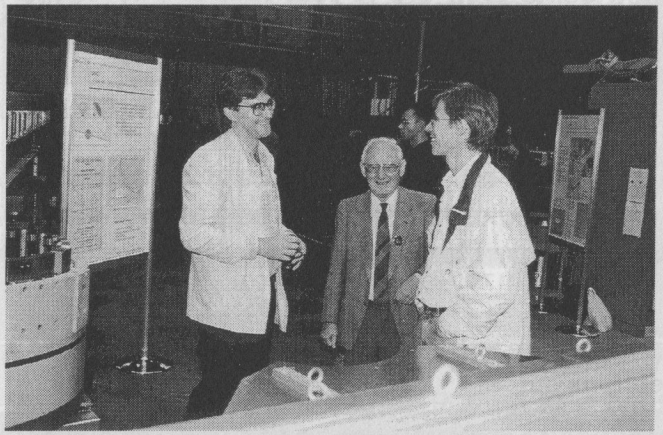
In the evening of the December 4 1996 we then rised the current up to approx 900 μA, corresponding to a beam power of about 520 kW. During this high power run we were able to test the shielding concerning the neutron- and gamma background, as well as the adequate function of cooling - and gas-containment circuits of target, moderator and in particular the cold neutron source.

After these satisfactory tests we plan to give to the source a "last" finish in order to start regular operation in Summer 1997 with four or five spectrometers attached to it.

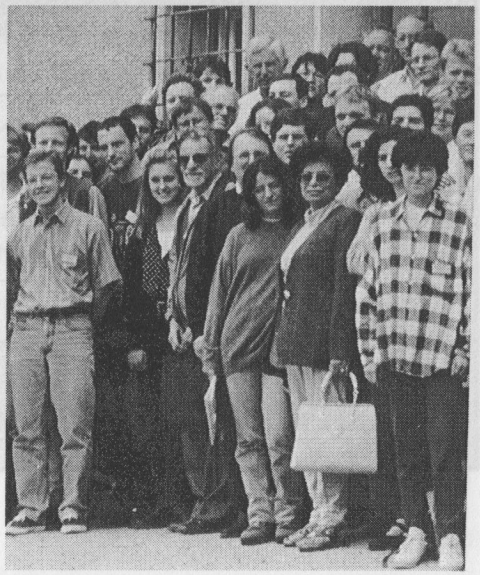


Gratulationen

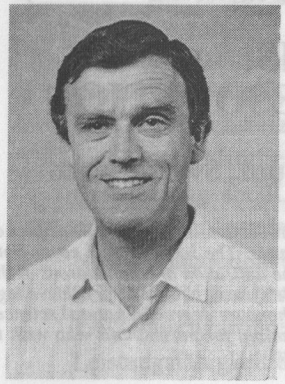
Unsere Ehrenmitglieder Prof. Dr. W. Hälg und Prof. Dr. K.A. Müller durften im April dieses Jahres ihren 80. und 70. Geburtstag feiern. Beide Jubilare sind nach wie vor aktiv mit der Schweizerischen Neutronenstreugemeinschaft verbunden, was die untenstehenden Fotos eindrücklich beweisen. Wir entbieten den Jubilaren unsere besten Glückwünsche für die Zukunft!



Prof. Dr. W. Hälg bei einem "Inspektionsbesuch" in der SINQ



Prof. Dr. K.A. Müller im Kreise der Teilnehmer an der Sommerschule über Neutronenstreuung in Zuoz



Der Lenkungsausschuss des **ILL (Institut Laue-Langevin, Grenoble)** hat an seiner Sitzung vom 29./30. Mai 1997 in Jülich den Vizepräsidenten unserer Gesellschaft,

Prof. Dr. Klaus Yvon
Université de Genève

zum neuen

Vorsitzenden des Scientific Council des ILL

gewählt.

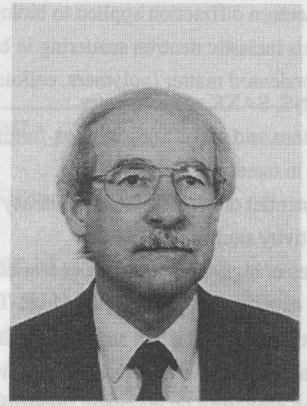
Das Komitee der **ENSA (European Neutron Scattering Association)** hat an seiner Sitzung vom 13./14. Juni 1997 in Florenz den Präsidenten unserer Gesellschaft,

Prof. Dr. Albert Furrer
ETH Zürich & Paul Scherrer Institut

zum neuen

Vorsitzenden der ENSA

gewählt.



Die Schweizerische Gesellschaft für Neutronenstreuung betrachtet diese Ehrungen, die mit viel zusätzlicher Arbeit verbunden sind, natürlich auch als Anerkennung ihrer bisherigen Aktivitäten zur Förderung der Neutronenstreuung. Sie gratuliert den beiden Gewählten und wünscht ihnen viel Freude und Befriedigung in ihrer neuen Aufgabe.

5th Summer School on Neutron Scattering

COLD NEUTRONS: LARGE SCALES - HIGH RESOLUTION

9-15 August 1997, Lyceum Alpinum, Zuoz, Switzerland

The main purpose of the Summer School is to give participants an introduction to the basic principles of neutron scattering and its application to the study of condensed matter. The lectures will cover both theoretical and experimental aspects. Particular emphasis will be on the utilisation of cold neutrons at the spallation neutron source SINQ at PSI, which enable to study large scale systems as well as to achieve high resolution. No previous knowledge of the subject is required, but an honours degree in natural sciences (equivalent to the diploma) is essential. A poster session will be organized for participants who wish to present their own results. The ***list of topics and invited lecturers*** *includes:*

Introduction to neutron scattering	*P. Böni, Villigen*
High-resolution neutron instruments	*S. Janssen, Villigen*
Polarized neutrons replace high resolution in particular cases	*B. Dorner, Grenoble*
SANS on double crystal diffractometer	*A. Ioffe, Berlin*
High-resolution SANS and spin-echo technique with focusing mirrors	*B. Alefeld, Jülich*
Elastic neutron scattering and hydrodynamics: Complementary methods for studying biological and macromolecular systems	*O. Byron, Leicester*
Cold neutron diffraction applied to biology	*T. Hauss, Berlin*
Towards inelastic neutron scattering in biology	*J. Zaccaï, Grenoble*
Soft condensed matter (polymers, colloids, microemulsions) by SANS, SAXS, reflectometry	*J.S. Pedersen, Risö*
Vibrations and relaxations in glass-forming polymers	*R. Zorn, Jülich*
SANS in materials physics	*P. Fratzl, Vienna*
The potential of off-specular reflectivity studies	*J. Webster, Didcot*
Reflectivity studies on fluids	*J. Als-Nielsen, Risö*
Vortices in high-temperature superconductors (tutorial lecture)	*J. Blatter, Zürich*
SANS experiments on vortices in high-T_C superconductors	*E.M. Forgan, Birmingham*
Excitations in normal and superfluid helium	*B. Fåk, Grenoble*
Anomalous phonons in $KTaO_3$ and $SrTiO_3$	*B. Hehlen, Montpellier*
Neutron scattering by magnetic fluctuations	*N. Bernhoeft, Grenoble*

Organization: R. Bercher (Secretary), W.E. Fischer (School Chairman), A. Furrer (Programme Chairman)

Residential accommodation will be available at the Lyceum Alpinum in Zuoz (costs: approximately 580 Swiss Francs, including full board, excursion, banquet, and Proceedings). The number of participants will be limited to 100. The language of the School is English. Closing date for applying is ***30 June 1997****. For further information and application forms, contact Renate Bercher, Paul Scherrer Institut, CH-5232 Villigen PSI, Tel.: +41-56-310 34 02, Fax: +41-56-310 32 94.*

The School is not yet booked out! Please apply immediately!

Mitteilungen

1. Das Schweizerische Bundesamt für Bildung und Wissenschaft hat unsere Gesellschaft beauftragt, im Hinblick auf die **Erneuerung des Vertrages Schweiz/ILL für die Periode 1999-2003** eine Umfrage unter den Mitgliedern zu organisieren, welche nicht nur die Entwicklung der ILL-Nutzung nach der Inbetriebnahme der SINQ voraussagen, sondern auch den Bedarf nach der Nutzung anderer Neutronenquellen (z.B. ISIS) abschätzen soll. Der Vorstand der SGN/SSDN hat beschlossen, diese Umfrage im September/Oktober 1997 durchzuführen, wenn erste Erfahrungen in Bezug auf die Leistungsfähigkeit der SINQ - im Quervergleich zu andern Quellen - vorliegen.

2. Die Projektstudie der **European Spallation Source (ESS)** liegt nun in gedruckter Form vor. Die Bände I (The European Spallation Source) und II (The Scientific Case) werden in den nächsten Wochen allen Mitgliedern unserer Gesellschaft zugestellt; der "dicke" Band III (The ESS Technical Study) kann von "Spezialisten" beim Sekretariat der SGN angefordert werden.

Vorankündigung

Freitag, 21. November 1997, am PSI Villigen, nachmittags:

Generalversammlung 1997 der SGN/SSDN

Die GV wird im Rahmen eines Workshops über

Powder Neutron Diffraction

abgehalten, welcher aus Anlass des

60. Geburtstages unseres Mitgliedes Dr. Peter Fischer

durchgeführt wird. Die Mitglieder der SGN/SSDN werden zu gegebener Zeit eine Einladung mit detailliertem Programm erhalten.

Zum Gedenken an Josef Benes

26. Dezember 1917 - 25. November 1996

Prof. Dr. J. Benes wurde in Vodnany in Südböhmen geboren, wo sein Vater Bahnhofvorstand war. Nach der Schulzeit begann er an der naturwissenschaftlichen Fakultät der Karls-Universität in Prag ein Studium mit den Hauptfächern Mathematik und Physik bei den Professoren Jarník und Zácek, wo er 1945 zum Doktor der Naturwissenschaften promovierte. Während der Kriegsjahre arbeitete er als Angestellter beim schwachstromtechnischen Konzern Ostmarkwerke in Prag. Aus seiner Jugendzeit sowie seiner Betätigung in der Industrie stammen seine Begeisterung für Eisenbahnprobleme und seine technisch-konstruktiven und handwerklichen Fähigkeiten.

Von 1945 bis 1968 war er an der Karls Universität Assistent, Oberassistent, Dozent und schliesslich ausserordentlicher Professor. 1947 studierte er während längerer Zeit am Nobel Institut bei Manne Siegbahn in Stockholm und wurde im Frühjahr 1948 an die physikalische Anstalt der Universität Basel delegiert, um dort den von mir aufgebauten Teilchenbeschleuniger für 1MeV Deuteronen kennen zu lernen. Prof. Petrsilka in Prag hatte eine gleiche Hochspannungsanlage bei der Firma Haefely bestellt, und Dr. Benes sollte sie später dort aufbauen. Aus dieser Zeit stammten unsere gemeinsamen freundschaftlichen Beziehungen.

Die Machtübernahme durch den Kommunisten Gottwald bildete das Ende der damals beginnenden Zusammenarbeit der Prager Forscher mit dem Westen. Sowohl Stockholm als auch Basel bemühten sich, dem jungen Benes eine Anstellung anzubieten und ihn davon abzuhalten in die Tschechoslowakei zurückzukehren, was er aber mit Rücksicht auf seine alleinstehende, von einer Staatspension abhängige Mutter ausschlug.

Erst zur Zeit des sogenannten Prager Frühling 1968 konnte der Kontakt mit Benes wieder aufgenommen werden. Ich vermittelte ihm eine Einladung zu einem einjährigen Forschungsaufenthalt bei der Delegation für Ausbildung und Hochschulforschung am Institut für Reaktortechnik der ETH Zürich. Kurz vor dem Einmarsch der Truppen der Sowjetunion gelang es ihm mit seiner Familie Prag noch zu verlassen. Diesmal hat er nach Ablauf des Gastaufenthaltes auf eine Rückkehr in seine Heimat verzichtet. Die ETH bot ihm eine Anstellung als Mitarbeiter in der Gruppe für Neutronenstreuung an. Seine pädagogischen Fähigkeiten konnte er im physikalischen Praktikum für Vorgerückte an der Abteilung für Physik und Mathematik auf dem Hönggerberg einbringen, wo er viele Studierende der Physik in die Kunst des Experimentierens einführte, und wofür er von der ETH 1975 zum Titularprofessor ernannt wurde.

Zur Technik der Neutronenstreuung hat er, seit deren Anfängen bei uns, beachtliche Beiträge geliefert, sei es in Form von umfangreichen Computerprogrammen zur Steuerung der Neutronenspektrometer, welche anfänglich noch in Maschinensprache geschrieben werden mussten, aber auch durch zahlreiche Konstruktionen von Spektrometerzusätzen, deren Fertigung und Inbetriebnahme er auf's sorgfältigste überwachte.

1982 erwarb J. Benes und seine Familie in Brugg AG das Schweizerische Bürgerrecht. Er hat sich sehr für die politischen Probleme seiner neuen Heimat interessiert und ist auch nach seinem Übertritt in den Ruhestand an Veranstaltungen, Seminarien und Kolloquien der ETH und des Laboratoriums für Neutronenstreuung ein treuer Gast gewesen. Er wird uns als Freund und Kollege in lieber Erinnerung bleiben.

Walter Hälg

Konferenzen 1997/98

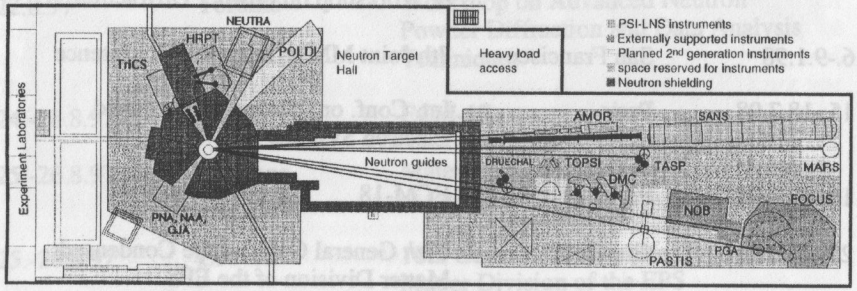
Datum	Ort	Thema
7.-11.7.97	Wollongong (bei Sydney)	THERMEC'97 (Synthesis, Processing & Applications of HTSC)
10.-20.7.97	Bialowieza	11*th* Int. Summer School of Cond. Matter
13.-17.7.97	Oxford	5th Int. Conf. "Surface X-Ray and Neutron Scattering"
14.-20.7.97	Eger, Hungary	3*rd* Summer School on High-Temperature Superconductivity
27.7.-1.8.97	Cairns	ICM'97
9.-15.8.97	Zuoz	5th Summer School on Neutron Scattering: "Cold Neutrons: Large Scales - High Resolution"
13.-15.8.97	Gaithersburg	Workshop on High-Resolution Cold Neutron Spectroscopy
15.-16.8.97	Upton	Satellite Symposium on Neutrons, X Rays, and Electrons: Complementary Tools for Structural Biology
17.-21.8.97	Toronto	ICNS'97
22.8.97	Toronto	Workshop on Advanced Neutron Powder Diffraction and Data Analysis Techniques
24.-28.8.97	Lisboa	ECM-17
25.-26.8.97	Argonne	Materials Research Using Cold Neutrons at Pulsed Sources
25.-28.8.97	Leuven	16th General Conf. of the Condensed Matter Division of the EPS
27.-31.8.97	Alpe d'Huez	Conference on Aperiodic Crystals

Datum	Ort	Thema
1.-12.9.97	Cargese, Corse	NATO ASI on the gap symmetry and fluctuations in HTSC
8.-18.9.97	Oxford	5th Summer School on Neutron Scattering
10.-12.9.97	Sacavem, Portugal	IAEA TCM on Neutron Beam Research Applications
14.-17.9.97	Kloster Seeon, D	Statusseminar: Neutronen, nukleare Sonden und Synchrotronstrahlung
14.-18.9.97	Cape Cod, Mass.	Spectroscopies in Novel Superconductors
14.-18.9.97	Paris	3rd Int. Conference on f-Elements
21.-26.9.97	Davos	Dynamical Properties of Solids
21.-26.9.97	Baden-Baden	Int. Conference Actinides '97
29.-30.9.97	Les Diablerets	Swiss Workshop on Superconductors and Novel Metals
2.10.97	Geneva	Annual Meeting SGK
10.10.97	Chaux-de-Fonds	Herbsttagung der SPG
21.11.97	Villigen PSI	General Assembly 1997 of SGN/SSDN & Workshop on Powder Diffraction
6.-9.1.98	San Francisco	7th Joint MMM-Intermag Conference
15.-18.7.98	Paris	Int. Conf. on "Strongly Correlated Electron Systems"
16.-20.8.98	Praha	ECM-18
25.-29.8.98	Grenoble	17*th* General Conf. of the Condensed Matter Division of the EPS
25.-28.10.98	Freemantle	International Rare-Earth Conference

Status of the SINQ-Instruments

P. Böni

In the contribution by W. Fischer you are informed that the Swiss spallation source SINQ at Paul Scherrer Institut was successfully run for the first time on December 3 and 4 1996. After the scheduled shut-down of the accelerator during January and February 1997, the spallation source was run again on March 21 and on May 6 1997 in order to do beam diagnostics and to test the radiation background.
In addition a monochromatic beam was extracted at the the three-axis spectrometer DrüchaL and the first Θ/2Θ-scans were conducted with pyrolytic graphite on the sample table. The first polarised beam experiment was performed using a Heusler monochromator, a remanent bender in front of the detector, and a flat coil spin flipper. All these experiments were done with a nominal proton beam current I=20μA during three hours.
The next SINQ-run at high currents is scheduled for July 1 1997 and we expect that during July the commissioning phase for some instruments can start on a more or less regular schedule.
On the following pages, spectrometer scientists provide the most recent information on the status of the first generation SINQ instruments (see also the figure below). For more details please consult World Wide Web on http://www1.psi.ch/www_sinq-hn/Welcome_SINQ.html. For preliminary experiments in fall 1997 you may contact the instrument scientists.



Irradiation Facilities for Thermal and Cold Neutrons at SINQ

E. Lehmann, G. Kühne

Designed for different applications, four irradiation facilities are under construction at the thermal beam port 60 in the target hall and at the end position of the neutron guide 13 in the neutron guide hall.

The rabbit system for **N**eutron **A**ctivation **A**nalysis will place small material samples at a neutron flux of 10^{12} to 10^{13} cm^{-2} s^{-1} for irradiation. After the exposure their content will be analysed with very high sensitivity and accuracy . From a chemistry laboratory which is located about 80 meters far from the irradiation position the samples are sent by air to a switch. There the sample is transferred to the inner irradiation circuit which is filled with helium.

About the same principle was used to built the facility for long term and high flux irradiation. The method is called **PNA** (Präparative Neutronenaktivierung) and will mainly be used to generate ^{111}Ag by exposing Pd. However, other irradiation can be performed for internal and external users if the limitations regarding the generated activity can be satisfied.

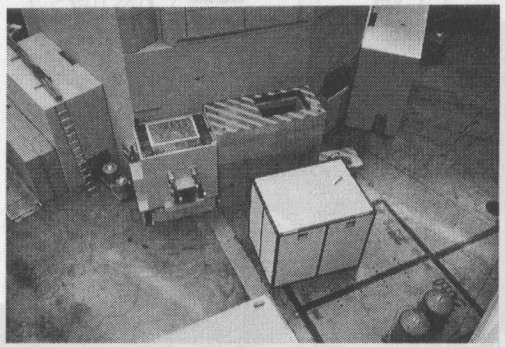


Figure: Transfer station (left), shielding room (at the target block) and control room (in front) as main components of the irradiation facilities. They will be completed and enclosed into one user laboratory during the second half of this year.

A gas-jet facility (**GJA**) is installed close to the surface of the moderator tank with three independent target chambers. The nickel foils with a thin layer of uranium-235 will be met by the neutron beam generating fission. The fission products are extracted and transported to a chemistry lab where they can be applied to several different experiments.

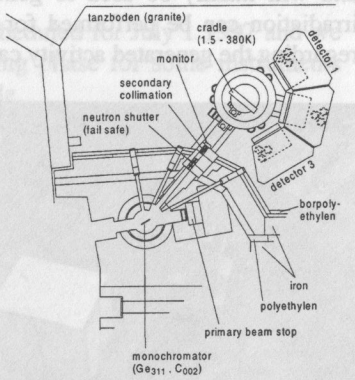
For special irradiation of medical and biological samples, mainly used in studies for **N**eutron **C**apture **T**herapy a shielded box is under construction and planed to be installed at the end position of the neutron guide 13. This remote controlled device will be very flexible and can be shared with investigations of the neutron radiography method using the intensive cold neutron beam.

Single Crystal Diffraction Instrument TriCS

J. Schefer
Laboratory for Neutron Scattering ETHZ&PSI, CH-5232 Villigen PSI

The TriCS is built as a good resolution single crystal diffraction instrument, covering the most often asked area between D9 and D19 at ILL. The operating mode is close to D19, the resolution between D9 and D19.
TriCS is using three area detectors on the basis of microstrip technology. The three area detectors have a fixed 2θ-difference, but may be positioned individually in height and distance to the sample. The tilting possibility allows to install almost any equipment on the instrument giving access to new experiments at extreme conditions e.g. in the field of magnetism and pressure. On the other side the temperature range between 1.5 K and presently 380 K is covered by our 4-circle equipment. Higher temperature could be made accessible. The TriCS will start service end of 1997.

wavelength λ	1.15 Å / 2.34 Å
monochromator	Ge311, PG002
take-off angle (2θ)	40.2°
tilting range γ	-5° to +40°
area detectors	He^3, microstrip
4-circle mode	1.5-380 K
tilting mode	7 mK - 1200 K
filters incoming	silicon,N_2-cooled
in pile collimation	none, 20', 40'



High Resolution Powder Diffactometer for Thermal Neutrons HRPT

P. Fischer, M. Koch and N. Schlumpf*, Laboratory for Neutron Scattering ETH Zurich & Paul Scherrer Institute*,CH-5232 Villigen PSI

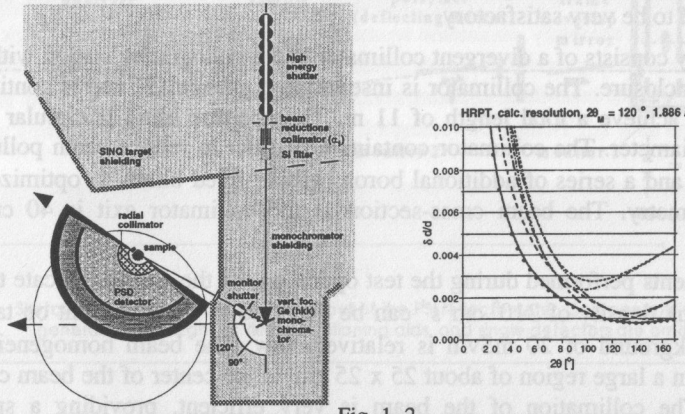


Fig. 1, 2

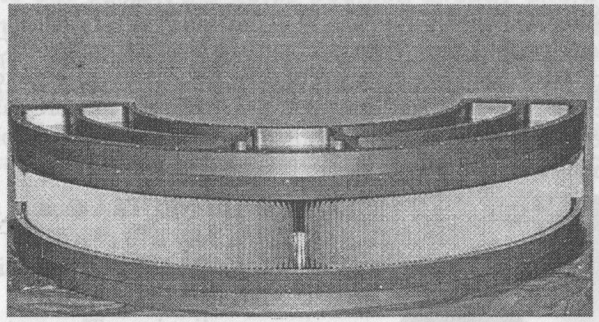


Fig. 3

Instrument properties: Best resolution $\delta d/d \leq 10^{-3}$ (in the high intensity mode $\approx 2.5 \times 10^{-3}$), d = lattice spacing. Neutron wavelength λ in the range from 1 to 3 Å (pyrolytic graphite filter for 2.5 Å). PSD LCP-1600-0.1° from Cerca: 1600 detectors (^{3}He) with angular separation 0.1° in a scattering angle range of 160°. The radial collimator with individually stretched mylar-Gd-O foils (Fig. 3) was made at Risø.
Status: In August the monochromator shielding, sample table mechanics and detector shielding of the instrument should be ready and first tests with the final prototype detector LCP-128-0.1° are planned. It is hoped that HRPT with vertically focusing wafer-type Ge monochromator and with the large detector will become operational at the end of 1997.

Neutron Transmission Radiography NEUTRA

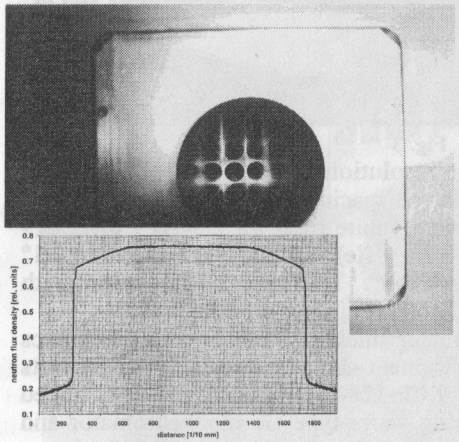
H. Pleinert and E. Lehmann, PSI

The NEUTRA facility will be operational in July 1997. First measurements have been carried out during the test operations of SINQ in December 1996 to determine the main beam parameters, and the performance of the facility has been found to be very satisfactory.

The facility consists of a divergent collimator and a radiography station within a shielded enclosure. The collimator is inserted into channel 32 and is continued outside to achieve a total length of 11 m. The aperture blind is circular with 2 cm of diameter. The collimator contains a Bi-filter to reduce beam pollution by γ-rays, and a series of additional boron carbide filled blinds to optimize the beam geometry. The beam cross-section at the collimator exit is 40 cm in diameter.

Measurements performed during the test operations of the source indicate that a thermal flux density of $2 \cdot 10^6$ $cm^{-2}s^{-1}$ can be expected at 1 mA current on target. The γ-background of 20 mSv/h is relatively low. The beam homogeneity is excellent in a large region of about 25 x 25 cm^2 at the center of the beam cross-section. The collimation of the beam is very efficient, providing a spatial resolution capacity down to structures of the order of 20 µm.

A set of detectors is being prepared, consisting of conventional Gd- and Dy / silver halide film sandwich detectors and of a CCD-based detector which has been developed at PSI and constitutes a state of the art instrument for measurements that require high quantitative precision. Imaging plates may be included in the future.

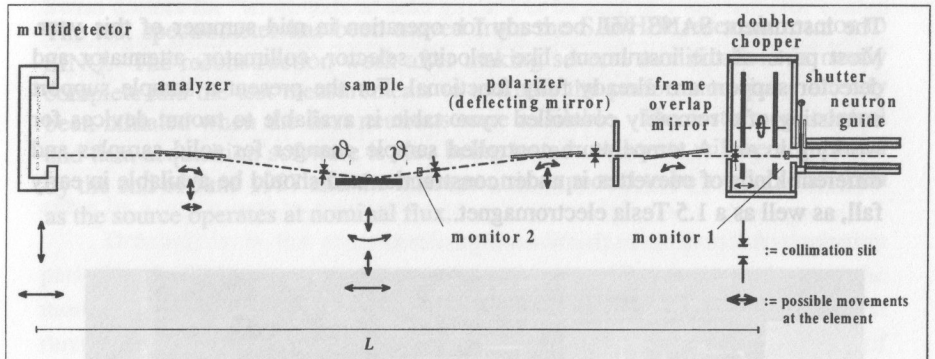


View into the beam channel where the profile of the neutron field was measured: the diagram shows the excellent homogeneity

The NEUTRA facility as completed in July will provide an efficient and flexible tool for a wide range of scientific and industrial applications. The next modification is currently in the planing phase and will be implemented at the end of 97, adding a specialized radiography station for investigation of highly radioactive samples.

Apparatus for Multi-Optional Reflectometry AMOR

D. Clemens, P. Gross, Paul Scherrer Institut, CH-5232 Villigen PSI



Sketch of the overall instrumental layout of the PSI reflectometer. Components for the generation of magnetic fields, positioning aids, and single detectors are omitted.

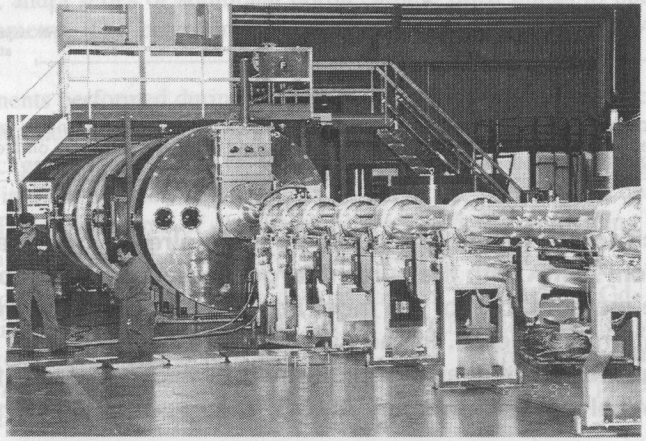
Very much to our delight the guide position already offers a mean flux of 1.3×10^8 *n*/cm²/s/mA with the current target according to Au foil irradition tests. At the moment, one of the most important and expensive parts, the chopper station is ordered. In the supermirror team we made successful developments for multilayer monochromators and polarizers that will be used as optical components on AMOR. Inauguration is scheduled for spring 1998.

bandwidth:	0.13 ... 1.3 nm
deflecting mirrors / polarizer	FeCoV/Ti:N supermirror, multilayer monochromator
collimation	0.05 ... 20 mm x 5 ... 55 mm
analyzer	FeCoV/Ti:N supermirror or FeCo/Si supermirror
detectors	^{3}He x-y-microstrip 172 mm * 190 mm and 2 ^{3}He single detectors
maximum sample size	150 mm x 500 mm
resolution	1.5% ... 10%
total length chopper-detector *L*	2.5 ... 10 m

Small Angle Neutron Scattering Instrument SANS

J. Kohlbrecher, W. Wagner, Paul Scherrer Institut, CH-5232 Villigen PSI

The instrument SANS will be ready for operation in mid summer of this year. Most parts of the instrument, like velocity selector, collimator, attenuator and detector support are already fully functional. For the present a sample support consisting of a remotely controlled xyzω table is available to mount devices for working in air. A temperature controlled sample changer for solid samples and different kinds of cuevettes is under construction and should be available in early fall, as well as a 1.5 Tesla electromagnet.



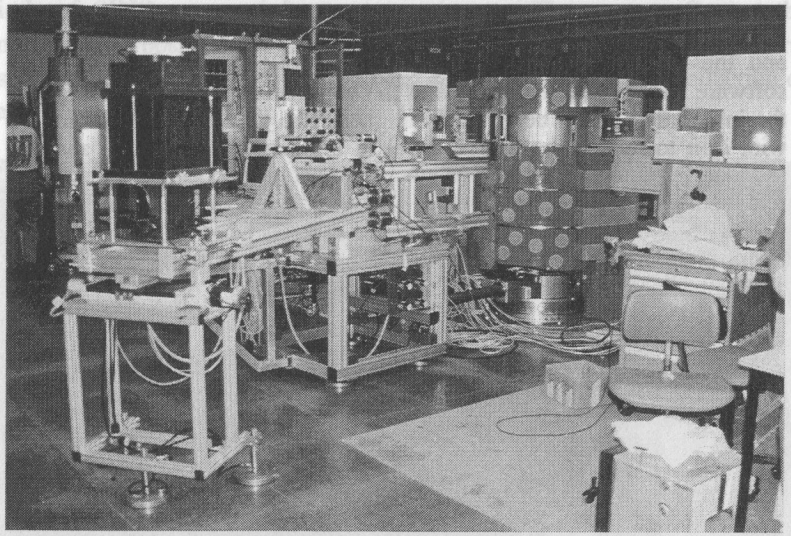
INSTRUMENT DATA

neutron guide	cold neutron guide, curved, Ni-coated, 50×50 mm^2
monochromator	helical slot velocity selector
wavelength	0.45nm $\leq \lambda \leq$ 4nm, resolution $\Delta\lambda/\lambda$=10 % (FWHM), variable by tilting
Q-range	6×10^{-3} nm^{-1} < Q < 10.5 nm^{-1}
detector	2D ^{3}He-detector, 128×128 elements of 7.5×7.5 mm^2, memory card to store 64 frames of 16k elements for time resolved measurements
collimation lengths	variable between 1 and 18 m
sample-detector distances	1.2 to 20 m continuously
lateral detector displacement	0 to 0.5 m

Two axis and neutron optics spectrometer at PSI, TOPSI

D.Clemens, M.Senthil Kumar, St.May and P.Keller
Paul Scherrer Institut, CH-5232 Villigen PSI

The test spectrometer has been moved from the SAPHIR research reactor to SINQ. The reconstruction work after making several modifications is nearly complete and the test measurements to evaluate the performance have already been initiated when the first neutrons were available. The instrument control and data acquisition software is also being tested. All tests will be completed by the end of June 1997 and the instrument is expected to be available as soon as the source operates at nominal flux.



Technical specifications:

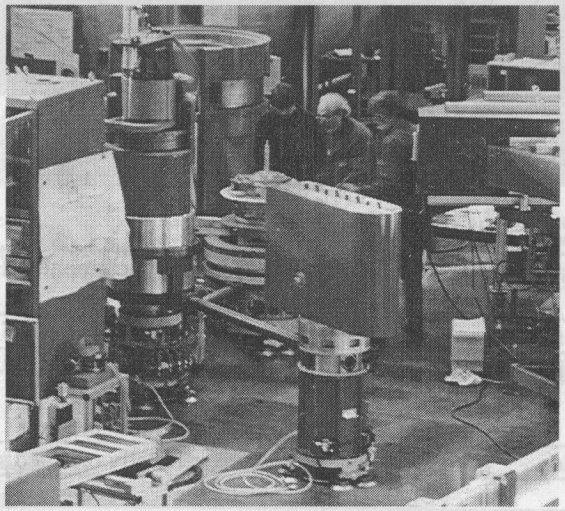
Monochromator	highly oriented pyrolytic graphite (HOPG) 2 theta(M) = 30° ... 145°
Collimation slits	dimensions (0.05 ... 35 mm) * (0.05 ... 55 mm)
Sample manipulation table	rotation (omega) 0 ... 360° (± 0.01°) tilt -20 ... 20° translation -40 ... 40 mm
Sample holder	yoke to pick up vertically oriented samples
Detectors	^{3}He single detector
Maximum sample size	500 mm * 150 mm * 100 mm

Three-Axis Spectrometer for Polarised Neutrons TASP

B. Roessli, P. Keller, and P. Böni, Laboratory for Neutron Scattering, ETHZ Zurich and Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

The three-axis spectrometer with full polarisation analysis option TASP is located at the end-position of the cold neutron guide 1RNR14. The monochromator take-off angles ($29° < 2\theta_M < 145°$) provides incident energies in the range $2\ meV < E_I < 30\ meV$. Neutron inelastic scattering is possible in the down scattering mode for a large range of energy transfers with an energy resolution varying between 7 μeV and 1 meV. An important advantage of the instrument is that almost all scattering angles are accessible in the W-configuration.

At present, the installation of the motor control units is in a final state and the instrument will be computer-controlled with the TASMAD software shortly. The monitors and the collimators are still missing and the instrument has to be optically aligned. The guide has been shielded with iron to reduce the gamma level in the experimental zone and the secondary beam-shutter is installed. Polarising benders composed of remanent supermirrors with m=3 and spin-flippers have been already successfully tested on the three-axis spectrometer DRÜCHAL. We hope, that full polarisation analysis on TASP can be performed in August 1997 after the installation of the guide fields.



TRIPLE-AXIS SPECTROMETER DrüchaL

Willi Bührer and Peter Keller

The triple-axis spectrometer DrüchaL ("**Drü**-achsigs am **chal**te **L**eiter", Swiss dialect for "triple-axis at cold guide") is located at a supermirror coated cold guide. Monochromator and analyser are equipped with pyrolytic graphite crystals. Options of vertical focusing and horizontal focusing on the monochromator and analyser respectively will give an enhanced neutron flux (at the expense of resolution). The electronics (hardware) is PSI standard, the software is an upgraded version of MAD-TAS. Instrument control can be made either by a labtop near by the instrument or from a cabin.

DrüchaL is in the process of commissioning: the low-flux operation periods of SINQ are used for test experiments. The neutron flux at the monochromator position is $\approx 2.6 \cdot 10^8\ cm^{-2}s^{-1}mA^{-1}$ (gold foil activation). First runs as a double-axis instrument have been performed on May 6 (production of polarised neutrons, test of supermirror benders).

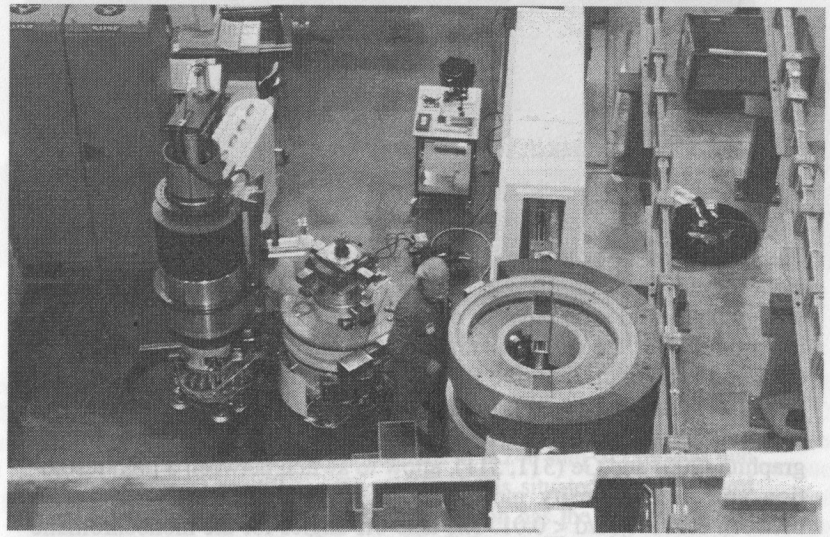


Figure 1: DrüchaL (seen from top along the neutron beam path)

incoming energy E_M	$2\ meV \leq E_M \leq 30\ meV$
sample	$-155° <$ scattering angle $< 155°$
typical energy resolution	$\Delta E \sim 0.01\ meV$ ($E_M = 2\ meV$)
	$\Delta E \sim 0.46\ meV$ ($E_M = 14.7\ meV$)

Cold Neutron Powder Diffractometer DMC

L. Keller
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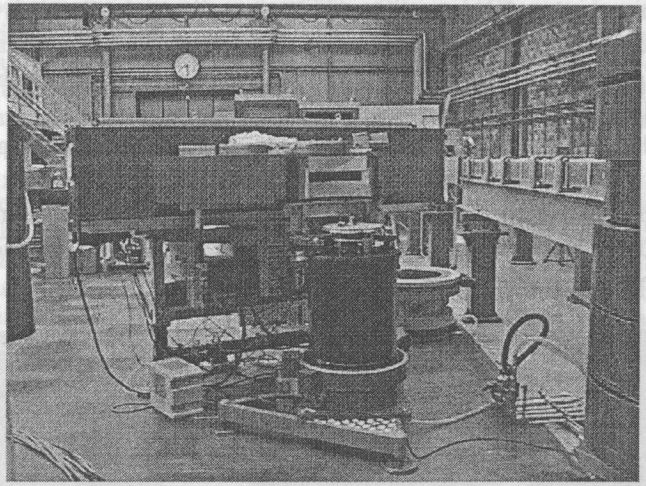

The Double-axis Multi-Counter diffractometer DMC is a flexible instrument for efficient neutron powder diffraction studies in the fields of crystallography, solid state physics, chemistry, material science and biology, in particular for the determination of weak magnetic intensities. Due to the use of a position sensitive BF_3 detector (400 detectors, angular separation 0.2°) simultaneous measurements within a scattering angle range of 80° will be possible. The two focusing monochromators, pyrolytic graphite (200) and Ge (311, 511), allow to switch between a high resolution and high intensity mode. The corresponding resolution varies between $0.001 < \delta d/d < 0.01$. The take-off-angles for the monochromatic beam can be varied between 30° and 135°. Standard measurements will be performed by means of an evacuated Vanadium pot equipped with a cooling machine. For experiments at very low temperatures cryostats are available. An oscillating radial collimator suppresses Bragg peaks from the sample environment such as cryostats or furnaces. An interesting option will be the use of polarised neutrons to separate ferromagnetic and nuclear intensities. The instrument will be operational with the focusing graphite monochromator in July, 1997.

Prompt gamma-ray activation PGA

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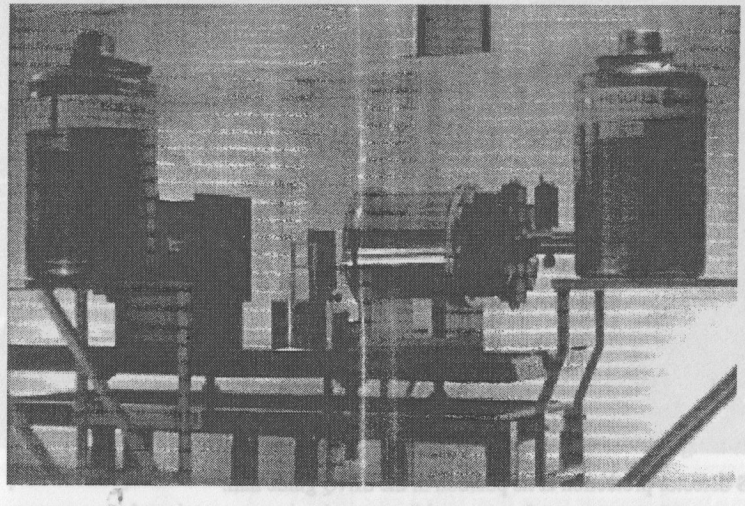
Prompt gamma-ray activation analysis (PGAA) is an excellent technique for determining the presence and quantity of elements in samples by the continuous irradiation with neutrons. The characteristic prompt gamma-rays, which are emitted following the neutron capture reaction by elements in the sample, will be observed simultaneously by two spectrometers (a Compton-suppression and a pair spectrometer).



The pair spectrometer (on the right of the above picture) consists of a 25 cm^3 Ge detector placed inside the central hole of a cylindrical NaI(Tl) scintillator of 254 mm in diameter and 254 mm in length, divided optically into six slices. The Compton-suppression spectrometer (on the left) is composed of a central Ge detector in a 240 mm SQ by 250 mm long NaI(Tl)/BGO scintillator. The BGO part is situated in the forward direction where the Compton-scattered radiation has the highest energy. The two detection systems were tested in Fribourg. The table supporting these two spectrometers, the sample holder and the neutron focusing lens, is already constructed. The neutron lens is composed of a large number of polycapillary fibres which are parallel at the lens entrance and are bent in such a way that all fibres converge towards a focal point. The diameter of the focused beam will be smaller than 1 mm and the flux gain will be greater than 30. The facility will be placed inside a concrete bunker. It will be necessary to shield the instruments against neutrons and to protect the scintillators from direct gamma radiation. The complete set-up will be installed by September 1997 at PSI.

FOCUS: Time-of-Flight Spectrometer for Cold Neutrons

S. Janssen[1,2], J. Mesot[2], L. Holitzner[1,2], R. Hempelmann[1]

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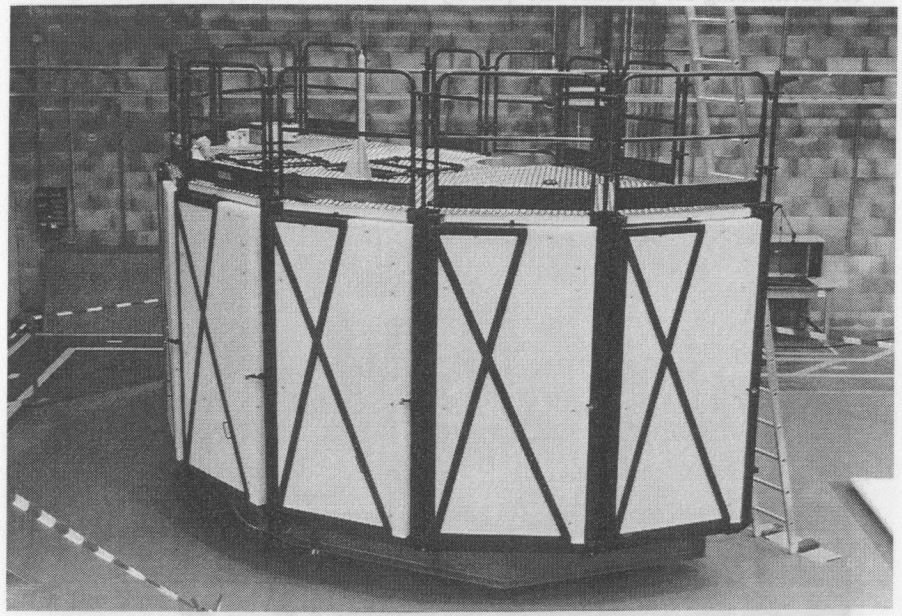

The FOCUS detector protection at its position in the SINQ guide hall.

In cooperation with the 'University of Saarbrücken' the Time-of-Flight Spectrometer FOCUS located at the end of the curved guide RNR11 is under construction. The concept of FOCUS consists in a hybrid-TOF that combines a doubly focusing crystal monochromator with a Fermi chopper. By means of variable distances between the main spectrometer components FOCUS can be operated either in time focusing or monochromatic focusing configuration, respectively.
The spectrometer allows for energy resolutions $\Delta E/E_i$ of 2-3% over a wide range of initial energies $0.3meV < E_i < 20meV$. Three detector banks cover a range of scattering angles from 10° to 130° providing a maximum achievable Q-value at E_i = 20meV of $Q = 5.6Å^{-1}$.
Meanwhile the detector protection with the sample line is installed on site (see photo). The other main components such as detectors, chopper system, and monochromator with its shielding are either already realised or under construction. After the test phase with neutrons FOCUS should go into its routine operation in summer 98.

The Mechanism of Hydrogen Diffusion in Nanocrystalline Palladium: a Quasielastic Neutron Scattering Study

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1. Introduction

It is a well known fact that changes of the interatomic distances within a crystalline structure cause interesting and different properties of the material. It can be achieved by the implementation of imperfections via thermal disorder with adjacent rapid freezing of the disordered state or by the employment of external tensions. In both cases the average atomic density of solids changes only slightly (within a few percent). On the other hand crystal imperfections as defects or grain boundaries cause drastic changes of the local atomic density. It is the basic idea of nanocrystalline materials to locate a large volume fraction of atoms within disordered regions by a strong reduction of grain size [1,2]. Nanostructured matter consists of polycrystals with grain sizes in the order of typically 5-50 nanometer. Hence the number of atoms located within defects such as internal surfaces or grain boundaries is comparable to those within the crystalline structure causing e.g. an enhanced mechanical strength of certain nanocrystalline metals or a ductile behaviour of nanocrystalline ceramic systems.
The mechanism of H-diffusion in coarse-grained and single crystalline Palladium has been intensively studied so far, see e.g. [3] and references therein. The great interest paid to the system is due to the fact that both diffusion rate and H-concentration show up proper values in a conveniently accessible range of pressures and temperatures. Especially the method of quasielastic neutron scattering (QENS) [4] has been applied successfully to gain microscopic understanding of the diffusion process of H in Pd. Sköld et al [5] showed from QENS experiments on coarse-grained Pd that Hydrogen performs a long-range diffusion via octahedral interstitials according to the well known Chudley-Elliot model [6].
Contrary, there is only few work done so far to investigate the properties of H in nanocrystalline Palladium. These studies focused on solubility measurements, vibrational properties, and macroscopic diffusion measurements [7-10]. Most prominent results were a shift of the solubility limit to higher H-concentrations and an increase of the chemical diffusion coefficient. It was found that a large fraction of Hydrogen is located within the grain boundaries of the material such that nanocrystralline PdH is an outstanding model system to investigate the diffusional properties of an interface-

dominated material. This study presents first tentative results that give insight into the microscopic mechanism of H-diffusion in nanocrystalline Palladium.

2. Experiments

Table I collects the relevant characteristics of the investigated samples. The parameters that have been varied during the experiments were temperature 'T', hydrogen content 'x', and the grain size 'd'. Samples were prepared using the technique of 'Pulsed Electrodeposition (PED)' [11] such that the necessarily large amount of sample material for neutron scattering experiments could be prepared within a reasonable time. The samples were of rectangular shape (height: 60mm, width: 25mm, thickness: 3mm) and were sealed after H-loading within an Al-container. From a variation of the sample thickness 'seen' by the neutron beam it could be excluded that effects of multiple scattering had to be considered.

sample	grain size d [nm]	Mass m [g]	H-content x [at-%]	T-range	instrument
1	45	11.3	3.7	160K - 330K	BSS, FZ Jülich
2	18	14.0	3.7	240K - 330K	BSS, FZ Jülich
3	12	26.2	3.7	240K - 300K	IN5, ILL

Table I: sample characteristics

The QENS experiments have been performed on the cold neutron 'Time-of-Flight' spectrometer IN5 at the 'Institut Laue Langevin' (ILL, Grenoble/FR) and on the backscattering spectrometer of the 'Forschungszentrum Jülich'/FRG. The Q-ranges of the spectrometers were $0.47Å^{-1} < Q < 1.80Å^{-1}$ and $0.16Å^{-1} < Q < 1.88Å^{-1}$, respectively. The combination of the two instruments allowed for the investigation of the H-diffusion within a broad dynamic range from $10^{8}s^{-1} < \omega < 10^{12}s^{-1}$.

3. Results

3.1 Backscattering

Figure 1 shows a representative result obtained from the backscattering spectrometer (BSS) on sample 2 (energy resolution: HWHM=0.7μeV). The data were corrected for scattering from the host lattice and the sample container. The solid line denotes a fit to the data with a single Lorentzian

$$S(Q,\omega) = \frac{1}{\pi}\frac{\lambda}{(\hbar\omega)^2 + \lambda^2}$$

folded with the measured instrumental resolution. The deviations below the figure exhibit the reasonable quality of the fit which indicates that a single diffusional process is observed. The obtained linewidths (λ=HWHM) are in the order of a few 'μeV'. In Figure 2 they are plotted as a function of the 'scattering vector Q at 4 temperatures for

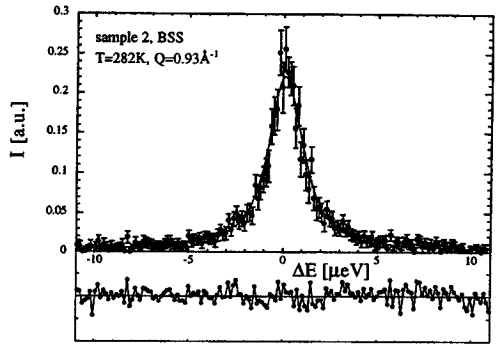

Fig. 1: QENS spectrum obtained from the backscattering spectrometer (BSS) at the FZ Jülich. The solid line denotes a fit with a single Lorentzian that provides a good description, see residuals below.

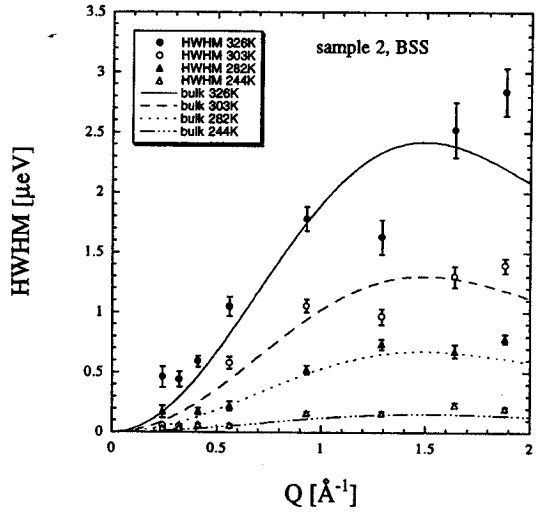

Fig. 2: Obtained linewidths for sample 2 as a function of Q. Solid and dashed lines denote a description with the isotropic Chudley-Elliot model and the literature parameters for coarse-grained PdH.

sample 2. The Chudley-Elliot model (CEM) [6] was originally developed to describe a liquid-like diffusion but could succesfully be applied to describe the H-diffusion in coarse-grained Palladium [5,3]. In terms of the CEM the linewidth is given by:

$$\lambda(Q,T) = \frac{6\hbar D}{l^2} \cdot \left\{1 - \frac{\sin(Ql)}{Ql}\right\}$$

'l' denotes the jump length and 'D' the diffusion coefficient whose temperature dependence is asumed to follow an Arrhenius law with activation energy E_A such as $D = D_0 \exp(-E_A/kT)$. A reasonable description of the data for all temperatures could be obtained with the prediction of the CEM and the respective literature values for coarse-grained PdH (E_A = 230mev, l = 3.0 Å) [3]. Just the prefactor of the effective diffusion coefficient turned out to be slightly more than one half of the coarse-grained PdH-value, namely (1.63 instead of 2.90)·10^{-3} cm^2/s. These results are represented by the solid and dashed lines within Figure 2. To study the size effects we performed QENS experiments on two samples with different grain sizes (18nm and 45nm, respectively, see Table I). Figure 3 presents the obtained linewidths at 3 temperatures that were identical within ±2K for both samples. As one can see within the statistical errors no effect of grain size is observable. The CEM-description of the linewidths is valid with identical results for both grain sizes.

3.2 Time-of-Flight (TOF)

The dynamic range of a cold neutron TOF-spectrometer such as IN5/ILL allows for energy transfers 100-1000 times larger than on a backscattering spectrometer. Therefore considerably faster diffusion processes can be analyzed. With a typical energy resolution HWHM of 30μeV a QENS experiment on coarse-grained PdH shows no line broadening beyond the instrumental resolution. Contrary, our TOF-experiments on nanocrystalline PdH revealed a significant quasielastic line-broadening that indicates a fast diffusional process not present in the coarse-grained reference material. Figure 4 shows a typical QENS spectrum obtained on sample 3 at T=300K. In total the range from 240-300K was investigated. For these spectra a description with a single Lorentzian was not sufficient indicated by the non-statistically distributed residuals above Fig. 4. However, as one can see from the decisive improvement of the residuals below the figure, a weighted sum of two Lorentzians reveals an excellent description of the data. Additionally, the fit included a comparatively large elastic contribution of more than 50% of the total scattering. It accounts primarily for the non-resolvable QENS-contribution visible by backscattering and secondly from elastic scattering arising from the host lattice and the sample container. Due to the tight schedule of beamtime no degased sample could be used as background reference here. The two quasielastic linewidths are clearly separated by a factor ~10 (broad component: 200-800μeV, narrow component: 20-100μeV).

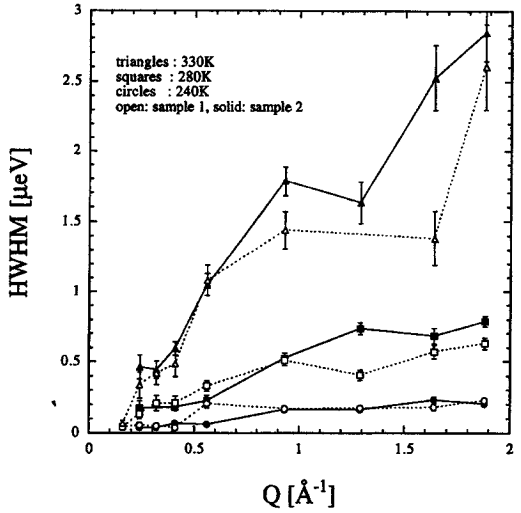

Fig. 3: Comparison of the quasielastic linewidths for two samples with different grain sizes (see Table I) obtained from backscattering.

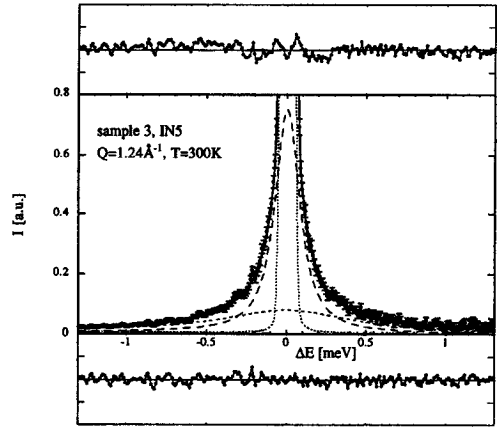

Fig. 4: Typical QENS-result obtained from TOF-spectrometer (IN5) for sample 3. A significant line broadening is observed that can be described by a weighted sum of two Lorentzians (solid line, residuals below the figure). The dashed lines denote the two quasielastic contributions as well as the remaining elastic contribution. A description with a single Lorentzian is not appropriate (residuals above).

The existence and the Q-dependence of the two observed linewidths combined with the Q-dependence of their relative weights triggered us to analyse the data in terms of a diffusion and trapping two-state model originally formulated by Singwi and Sjölander [12]. It could be successfully applied to describe e.g. the mechanism of Hydrogen diffusion in N-doped Nb [13], in amorphous $Pd_{85}Si_{15}H_{7.5}$ [14], and of the proton diffusion in Yb-doped $SrCeO_3$ [15]. The model asumes a long range diffusion via a random walk of the Hydrogen atoms over the regular H-sites with the jump rate $1/\tau$ and a jump length 'l' according to the isotropic CEM. After a mean time τ_1 the H-atoms meet deep local minima of the single particle H-potential, so called 'traps' with a mean distance 's' to each other. The origin of those traps will be discussed in the next chapter. The mean residence time within a trap is τ_0, such that $1/\tau_0$ and $1/\tau_1$ are called escape and trapping rate, respectively. For further theoretical background see [13,15].

Figure 5 shows exemplarily the IN5-result for sample 3 at T=269K and different Q-values together with a fit with the two state model. Totally, 8 spectra over the entire Q-range were simultaneously fitted for each temperature. As one can see a good agreement is achieved. The respective χ^2-values were 1.23(240K), 1.22(269K), and 1.37(298K).

Figure 6 finally shows the result for the temperature dependence of the three jump rates. The respective activation energies for the trapping rate $1/\tau_1$ and the free diffusion jump rate $1/\tau$ are both close to 200meV, wheras the escape rate $1/\tau_0$ is more than twice as big (440meV) in agreement with the two state model. Table II collects the temporal and spatial parameters of the diffusion mechanism obtained from the model dependent data evaluation.

Parameter	T=240K	T=269K	T=298K
$1/\tau$ [s^{-1}]	$(2.4\pm0.2)\cdot10^{11}$	$(4.6\pm0.4)\cdot10^{11}$	$(1.7\pm0.2)\cdot10^{11}$
$1/\tau_1$ [s^{-1}]	$(9.1\pm0.9)\cdot10^{9}$	$(2.0\pm0.2)\cdot10^{11}$	$(7.6\pm0.8)\cdot10^{11}$
$1/\tau_0$ [s^{-1}]	$(5.0\pm0.8)\cdot10^{9}$	$(9.5\pm1.5)\cdot10^{11}$	$(3.0\pm0.3)\cdot10^{11}$
D_{eff} [cm^2/s]	$(2.0\pm1.0)\cdot10^{-6}$	$(4.1\pm2.0)\cdot10^{-6}$	$(1.4\pm0.8)\cdot10^{-5}$
jump length l [Å]		0.8±0.4	
mean free path s [Å]		3.8±1.8	

Table II: Temporal and spatial parameters for the fast H diffusion in nanocrystalline PdH.

Furthermore experiments were performed on the ILL-backscattering spectrometer IN16 and on IN5 on samples that were prepared by the treatment of 'Inert Gas Condensation (IGC)' [16,17]. Those samples were loaded with slightly less Hydrogen (2.9 at-%). In both cases the results were qualitatively in agreement with the data from PED-samples, but the low total mass of the IGC samples causing statistical problems for the QENS-experiments rendered more difficult a precise quantitative analysis of the data.

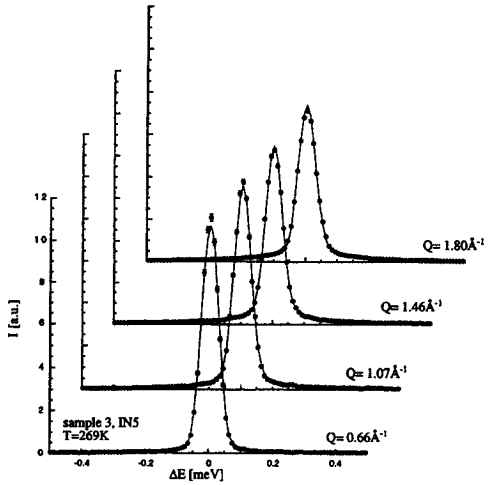

Fig. 5: QENS data at various Q-values together with the result of the simultaneous fit with the two-state model. In total the fit included 8 spectra for each temperature.

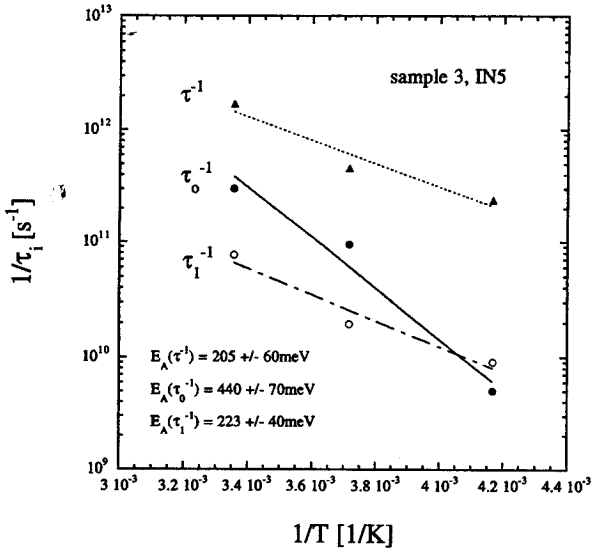

Fig. 6: Temperature dependence of the jump rates obtained from the simultaneous fits. As expected the activation energy for the escape rate $1/\tau_0$ is significantly higher than those of $1/\tau$ and $1/\tau_1$.

4. Discussion

From the results presented in the previous chapter one can deduce that there are two microscopic mechanisms that are responsible for the H-diffusion process in nanocrystalline Pd.

First, within the nanocrystalline grains the diffusion process is very similar to coarse-grained PdH (backscattering-results). The H-atoms perform a long range diffusion (compared to their jump length) via octahedral intestitials within the regular Pd lattice. Activation energy and jump length are identical to the one found for the coarse-grained material. Due to a reduced prefactor D_0 the Diffusion coefficient is slightly smaller for the nanocrystalline Pd. Besides that no confinement effects due to the strongly reduced grain size could be detected. Even for our smallest grain size of 18nm the crystalline regions are still large compared to the jump length (0.3nm) of the diffusion process.

Secondly, the TOF-results exhibit a second diffusion process that is not present in the coarse-grained material. We attribute this process to a fast H-jump mechanism within the grain boundaries of the structure that is hindered by certain H-traps. At T=300K the jump rate for the diffusion in between the traps is $1.7 \cdot 10^{12}$ s^{-1} that is 500 times faster than in coarse-grained PdH and even 15 times faster than in the entirely amorphous $Pd_{85}Si_{15}H_{7.5}$ [14], where the mechanism of H-diffusion could be explained with the same two-state model as applied in the present study. A strong experimental hint on the existence of traps can be deduced from the effective diffusion coefficients D_{eff}. Compared to coarse-grained PdH where no trapping occurs the factor in D_{eff} drops from 500 to ~30, whereas the ratio of D_{eff} between amorphous $Pd_{85}Si_{15}H_{7.5}$ and nano-PdH is still close to 15, because in both cases traps affect D_{eff}.

Furthermore, we obtained a remarkably small mean jump length with a value less than 30% of the one found in a regular Pd host lattice. Also for amorphous $Pd_{85}Si_{15}H_{7.5}$ a small jump length of 1.75Å was found [14]. Experimental hints exist that the degree of atomic short range order within the grain boundaries of nanocrystalline solids can even be lesser than in a purely amorphous substance [18]. Thus a reduced jump length might be a property of a non-regular host lattice. Nevertheless one has also to consider the possibility of an artefact due to the circumstance that Q_{max} was limited to 1.8Å^{-1} and hence the experiment is not sensitive to distances in the order of 1Å.

Considering the origin of the trapping sites one can either think of sites located just below the surfaces of nanocrystalline grains, so called subsurface sites, or of impurities which are due to the preparation process. From hot extraction analysis it is known that nano-Pd samples obtained from the PED-process contain significantly more 'O'- and 'N'-impurities than standard Pd-samples [11]. Dependent on the grain size the PED-prepared samples imply between 1 and 2 at-% 'O'-impurities which are concentrated mainly within the grain boundaries. Thus a possible explanation is the existence of highly electronegative 'O'-impurities that cause deep local minima of the effective

single particle H-potential. Another hint on the impurity origin of the traps is the ratio of the activation energies of $1/\tau_0$ and $1/\tau_1$ that is 2.0 and thus identical to the one found for Yb doped $SrCeO_3$ [15]. These arguments favour the impurity caused H-traps but for a detailed explanation further studies have to be performed.

5. Conclusions

The microscopic mechanism of H-diffusion in nanocrystalline PdH has been studied using QENS in a broad dynamic range over more than four orders of magnitude in energy. Our tentative results showed that the diffusion mechanism within the nanocrystalline grains is almost identical to the one found in coarse-grained PdH. Besides that a fast diffusion process has been observed that is not present in ordinary PdH systems. It is caused by the diffusion within the grain boundaries of the material and can be described consistently with a diffusion and trapping two-state model. Thus the fast diffusion process is an inherent property of the nanocrystalline structure. It is caused by the large fraction of grain boundaries and disordered domains.

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