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High-resolution powder diffractometer HRPT for thermal neutrons at SINQ

P. Fischer[a,*], G. Frey[a], M. Koch[a], M. Könnecke[a], V. Pomjakushin[a], J. Schefer[a], R. Thut[a], N. Schlumpf[b], R. Bürge[b], U. Greuter[b], S. Bondt[b], E. Berruyer[c]

[a]*Laboratory for Neutron Scattering ETH Zürich and Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*
[b]*Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*
[c]*Cerca, F-26100 Romans, France*

Abstract

Design characteristics and first experience concerning the new high-resolution powder diffractometer for thermal neutrons at the Swiss spallation neutron source SINQ are summarized. It is based on a linear position-sensitive ^{3}He detector with 1600 wires and angular separation of 0.1°, permitting also real-time experiments.

Keywords: Neutron instruments; Powder diffractometer; Position sensitive detectors; Monochromators

The neutron powder diffractometer for thermal neutrons at the target station of the Swiss continuous spallation neutron source SINQ (Fig. 1) is designed as a flexible instrument for high-resolution [best values $\delta d/d$: $(<1, <2)\times 10^{-3}$ with d being the lattice spacing in the high-resolution or high-intensity modes, respectively]. The neutrons originate from a H_2O scatterer close to the SINQ target and pass a liquid nitrogen cooled Si filter of 20 cm length. The diffractometer uses large scattering angles $2\theta_M = 120°$ or 90° of the monochromator. Intensity gains up to a factor of 4 are achieved by means of a 28 cm high, vertically focusing wafer-type Ge ($h\,k\,k$) monochromator with variable curvature (Fig. 2). A position-sensitive ^{3}He (3.6 bar + 1.1 bar CF_4) detector (radius 1.5 m, active height 15 cm) is used. It was produced by Cerca at Romans, France and has 1600 (25×64) wires with an angular separation of 0.1°. Fig. 3 shows the excellent detector characteristics. Modern electronics for the 25 modules including a central data exchange PC system, an external Cerca PC, the PSI interface and histogram memory were developed by E. Berruyer, Cerca and by PSI. A special cooling system had to be installed for the detector electronics producing about 1 kW of heat.

The SICS software of PSI controls the instrument with a server running on a unix workstation and clients written in Java through the TCP/IP network.

Primary Gd–O Soller collimation ($\alpha_1 = 6'$, $12'$ or open $\approx 40'$) and a secondary slit system enable to tune the instrumental resolution to the needs. Depending on the Ge ($h\,k\,k$) plane used, neutron wavelengths in the range from approximately 1–2.5 Å may be chosen. An oscillating radial collimator consisting of individually stretched mylar foils coated with Gd–O (Fig. 4) removes Bragg peaks from the sample environment. It was fabricated by J. Linderholm (JJ X-Ray) at Risø.

Complementary to synchrotron X-ray powder diffraction studies the applications of HRPT will be high-resolution refinement of chemical and magnetic structures as well as phase analysis, the detection of defects and internal microstrain. Also real-time investigations of chemical or structural changes and of magnetic phase transitions in crystalline, quasicrystalline, amorphous and liquid samples including technically interesting new materials are possible for a temperature range from approximately 50 mK to 2100 K, and hydrostatic pressures up to 12 kbar will be accessible.

* Corresponding author. Fax: + 41-56-310-2939.
E-mail address: peter.fischer@psi.ch (P. Fischer)

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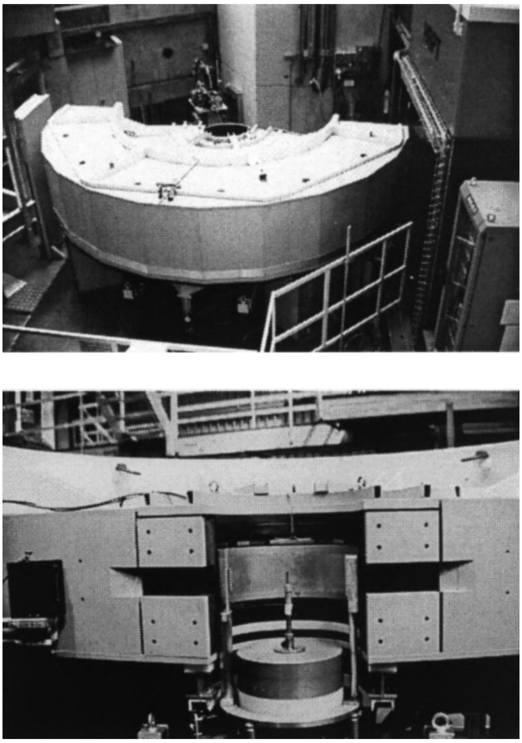

Fig. 1. HRPT at SINQ target station.

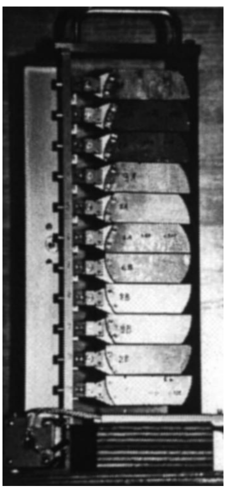

Fig. 2. Wafer Ge monochromator of HRPT.

First results obtained on HRPT with step 0.05° and resolution $\delta d/d$ of the order of 0.002 [see insertion for Si ($\phi = 10$ mm)] are shown in Fig. 5.

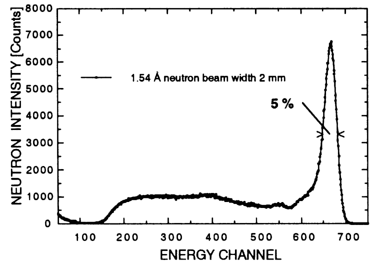

Fig. 3. HRPT detector characteristics.

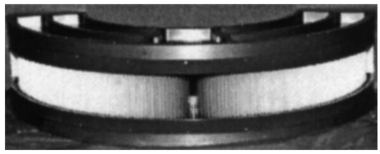

Fig. 4. Radial collimator of HRPT.

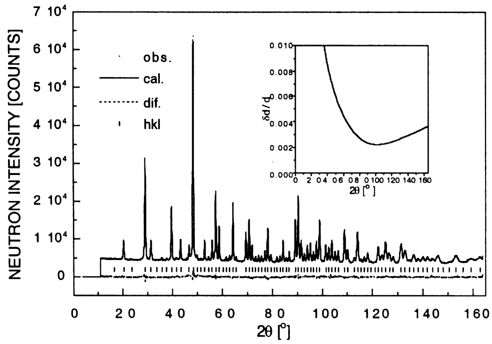

Fig. 5. Observed and calculated neutron diffraction patterns of Y_2O_3 ($\phi = 8$ mm, lattice parameter $a = 10.613$ Å, space group I a 3) for $\lambda = 1.539$ Å, $2\theta_M = 90°$, collimations $\alpha_1 = 12'$, $\alpha_2 \approx 24'$.