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Installation of the high resolution TOF diffractometer at the Budapest Research Reactor

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Abstract. The new TOF project started in 2000 in collaboration with the Hahn-Meitner-Institut. The spectrometer - previously tested on a cold beam - has been reinstalled to a radial thermal neutron beam at the Budapest Research Reactor. The TOF monochromator system consist of a double chopper with maximum rotation speed of 12000 rpm and the two single ones with 6000 rpm. The instrument will operate with a 2-dimensional detector of $80x100cm^2$ in back scattering geometry, now He^3 tubes are used. The first test measurements we are presenting here show that the expected resolution $\Delta d/d \sim 4x10^{-4}$ can be achieved.

Introduction

In 1996 the instrument was installed at a cold beam for testing the efficiency of time of flight (TOF) spectroscopy on a long-pulse spallation source [1]. According to the Monte-Carlo simulation results [2-3] it was expected that this type of instrument can outperform a conventional powder diffractometer at continuous reactor source in the resolution range of $\Delta d/d = 1–5\times10^{-3}$. The other advantage to apply TOF monochromatisation to neutron diffractometry on a continuous source is the variable resolution and intensity. A full diffraction spectrum can be gained within a variable bandwidth with ultrahigh resolution or with high intensity at conventional resolutions. Taking considerations of these aspects, the instrument has been rebuilt as a user instrument at a thermal beam in a new guide hall and became ready for tests in September 2005 [4].

Discussion and results

Instrument description

The double disk chopper (Ch1 and Ch2) has two windows: a 1.5° opening for short pulses (10 μs) and a 15° window for long variable pulses (20–200 μs), and can be operated in parallel or counter rotating mode. The latter option is used to produce very short pulses at high speed. To minimize the opening time the neutron beam is reduced from 25 to 10 mm width at the position of the pulse choppers using a 4.5m compressor neutron guide section before and a same decompressor after them (see Fig.. 1). Ch3 limits the crosstalk between different pulses and Ch4 prevents frame overlap. Although the coating of the choppers starts to transmit short wavelength below 0.07 nm, the neutron guide is straight to keep more short-wavelength neutron in the beam. Unfortunately this causes relatively high background in the spectra but it can be reduced using better beam stop geometry. The total number of thermal neutrons at the sample positions in the beam is about $2x10^9$ per seconds if all the windows are open.

The instrument is working in back scattering mode to reach the best possible resolution. Until the planned detector (a 60x100 cm^2 2D detector) reach completion, a box of four He^3 tubes is used with a 3kHz Event Recording Board. Because of the much smaller surface, the box is placed closer (1.5-2m) to the sample. To achieve the maximum resolution the 2D position sensitive detector will be needed.

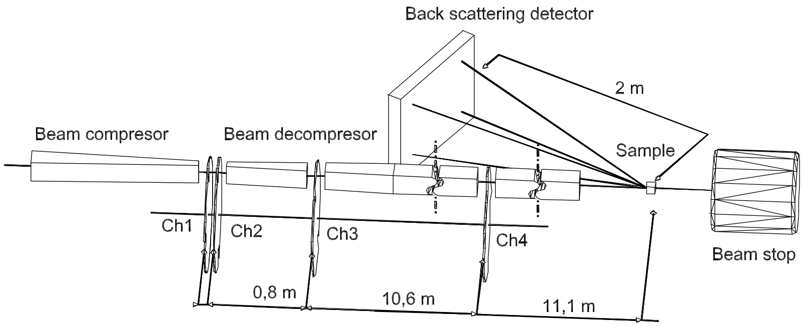

Figure1. Instrument Layout

Table 1. Instrument data.

Total flight path from chopper 1	L=26.5 m
Bandwidth Δλ	from 0.3 nm (beam spectrum) to 0.08 nm (200 Hz)
Resolution Δd/d	$1x10^{-3}$ at l=0.1 nm
Straight neutron guide cross section	25x100 mm^2 - (10x100 at Ch12)
Coating	Supermirror NiTi, m=2
Flux at opened windows at the sample	$8x10^7$ neutron/s/cm^2 (th. eq. flux)
Chopper disk inner and outer diameters	500 mm - 700 mm
Space between disks 1 & 2	27 mm
Material and coating	Carbon fibre epoxy - Gd_2O_3
Max. speed for 1 ,2 and 3,4	12000 rpm - 6000 rpm
Detector size and angle	600x1000 mm^2 - 160°-170°

Resolution tests with powder and single crystal samples

The resolution of a TOF monochromator system is given by the equation:

$$(\Delta d/d)^2=(\Delta t/t)^2+(\Delta L/L)^2+(\Delta\Theta/\tan(\Theta))^2. \quad (1)$$

In backscattering mode with 2D detector the last term can practically be eliminated, only the used beam cross-section limits it. The path length uncertainty is determined by the sample and detector thickness and can be somewhat less then $1x10^{-3}$ in our case. The first term is wavelength dependent. Since the shortest pulse is 10μs this term takes $0.7x10^{-3}$ at λ=2Å. All this means that Δd/d=0.001 for d=1Å, and can be even better, $5x10^{-4}$ for d=2Å.

The test measurements were carried out on a sintered alumina (Fig. 2) as powder sample and on Si111 wafers (Fig. 3) as single crystal. Both experiments confirm that the instrument is capable for high resolution measurements at very good intensity already in its present state. Thanks to the stability and precision of the chopper and detector system the sensitivity for line broadening can be at least one order of magnitude better, i.e. $1x10^{-4}$. In the second case two packs of wafers were placed in Bragg position with different distance from each others. These spectra demonstrate how close peaks can still be distinguished. For the single crystal, the peaks fall apart above $1x10^{-3}$Å already and it is not worse than in the case of powder sample: The (1,1,9) and (1,0,10) reflections of Al_2O_3 can be completely unfolded (upper part of Fig. 2) while at four times worse resolution and in “one detector mode” one can only see a shoulder (lower part).

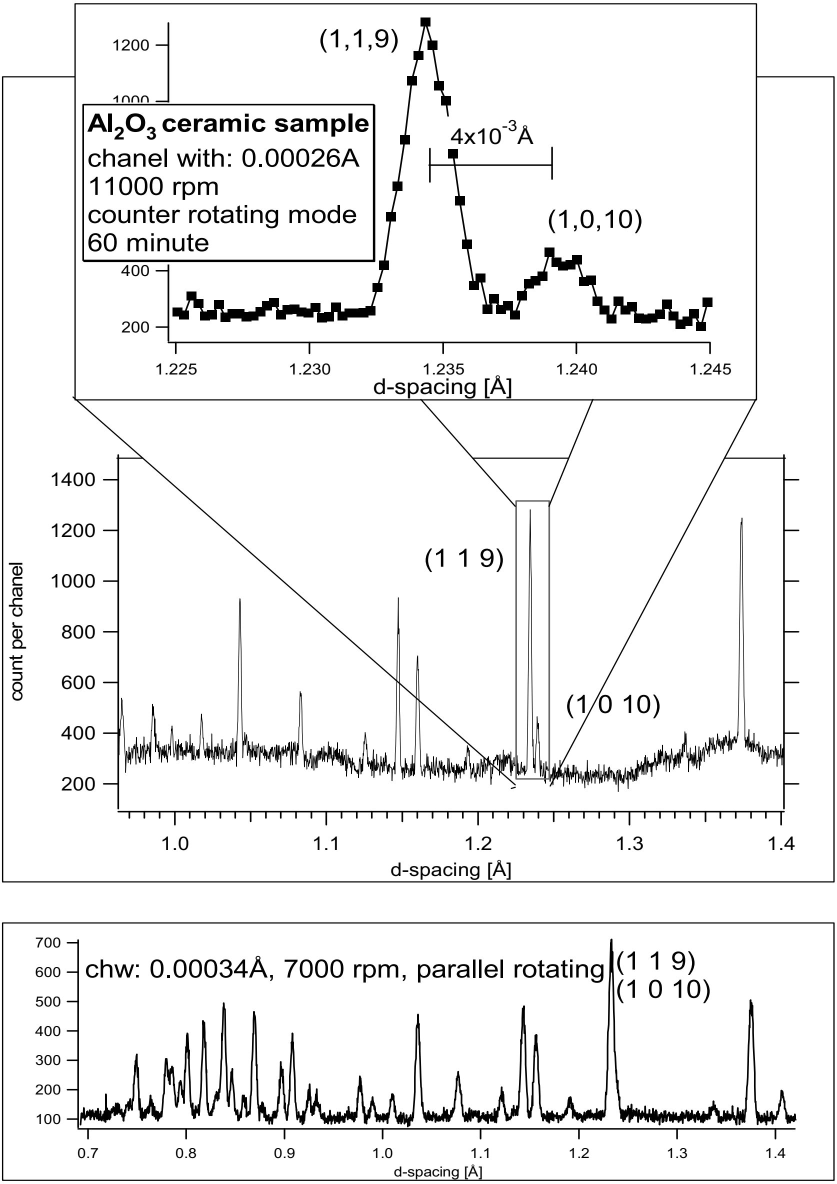

Figure 2. Resolution test with powder sample. Diffraction spectra from 8cm^3 sintered Al_2O_3 at low (below) and high resolution mode (above).

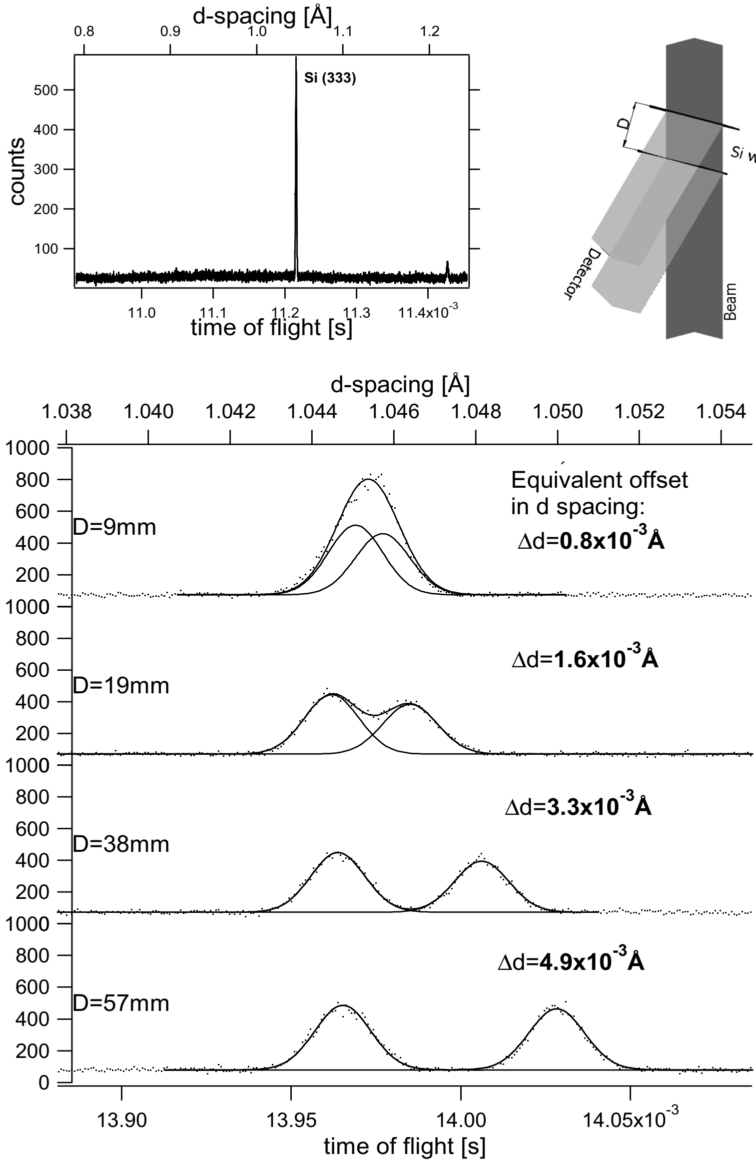

Figure 3. Resolution test with Si single crystal wafers. Two 3mm thick wafer pack was measured with different spacing between them. The solid lines are the fits to the Gaussian functions.

Conclusions

The TOF diffractometer installed at the Budapest Research Reactor became available for real experiments. The good intensity and high resolution ($\Delta d/d=0.001$ for $d=1$Å) is demonstrated. The monochromator system is in final state but the planned large surface 2D detector will be necessary to operate with the full capacity. The relatively strong background can be reduced even by single crystal filter as well as by using borated chopper disks or both if the problem can not be fixed at the beam stop.

References

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