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FOURIER RTOF DIFFRACTOMETERS

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Structural investigations of matter can be performed effectively by thermal neutron scattering using a time-of-flight (TOF) diffractometer which for the first time was realized by B.Buras et al. at the steady state reactor in Warsaw in 1966 and at the IBR pulsed reactor in Dubna in 1964. A conventional TOF diffractometer at a pulsed neutron source with a narrow neutron pulse can provide high resolution at a reasonable neutron flux on the sample. In the case of a steady state neutron source or a pulsed neutron source with a large (> 100 μs) neutron pulse duration conventional TOF diffractometry is not an effective way of using the available neutron flux. In this case a Fourier chopper can be applied to provide a more economical use of available neutron fluxes without loss in resolution.

General ideas of neutron Fourier diffractometry were considered by J.F.Colwel, P.H.Miller and W.L.Whittemore in 1968. This technique involves neutron beam modulation by rotating a disk with a pattern of alternating neutron absorbing and neutron transparent slits which ensures little loss in neutron intensity. In this case, spectrum refinement requires exact knowledge of the phase of the chopper at the time the neutron wave passes through it. Solution of this problem in the form of the reverse TOF method (RTOF method) was proposed by P. Hiismäki in 1972.

The basic idea of the RTOF method is to check, for each detected neutron, whether certain postulated neutron histories have a high or low probability of occurrence on the basis of a knowledge of the actual state of the source or of the time-dependent selectors installed on the flight path. Because the detection of a neutron takes place at the very end of its flight, checking must extend from the instants of the immediate past all the way to the longest TOF expected. Therefore, the history of the state of the source and of the neutron selectors must be made available as contiuously updated arrays for real time classifications between the high or low probability histories. Such arrays are conventioanlly obtained from discrete electronic correlators which are essentially the time-shift registers provided with parallel outputs for every time channel.

The RTOF method was demonstrated at the low power steady state reactor of VTT in Espoo, Finland in 1975. In 1984, the first Fourier RTOF diffractometer, mini SFINKS, was constructed at the 16 MW reactor of PNPI in Gatchina, Russia, in collaboration with a group from Finland. The experience of the Gatchina group was utilized at the 5 MW reactor of GKSS in Geesthacht, Germany, where a specialized Fourier Strain Spectrometer (FSS) was constructed in 1988. A basic step forward was the construction of the HRFD high resolution Fourier diffractometer at the IBR-2 high flux pulsed reactor in Dubna, Russia. It was the first implementation of such a diffractometer at a pulsed source with a relatively long pulse. The

IBR-2 reactor is the most intense pulsed source in the world with a peak flux of 10^{16}n/cm^2/s and pulse width of 320 μs for thermal neutrons.

To illustrate the gist of the Fourier RTOF method, let us consider the spatial resolution of the TOF diffractometer

$$R = \Delta d/d = [(\Delta t/t)^2 + (\Delta\theta/\mathrm{tg}\theta)^2]^{1/2},$$

where Δt is the neutron pulse width, and $t \sim L \cdot d \cdot \sin\theta$, θ is the scattering angle. We have several possibilities for improving the resolution: $R \to 0$ at $\Delta t \to 0$ or $L \to \infty$ and $\Delta\theta \to 0$ or $\theta \to \pi/2$.

A usual TOF diffractometer can give high resolution for a fixed narrow pulse at a large distance from the source, as in the case of HRPD at ISIS: $\theta \to \pi/2$, $\Delta t \approx 12$ μs, $L = 100$ m, $R = 5 \cdot 10^{-4}$.

The Fourier RTOF diffractometer produces a narrow pulse from an initially long pulse: $\Delta t \approx \Omega^{-1}_{m}$, the inverse maximum frequency of neutron beam modulation, and can give high resolution at a minimal distance, as in the case of HRFD at IBR-2:

$\Delta\theta \to 0$, Δt (reduced) ≈ 7 μs, $L = 20$ m, $R = 5 \cdot 10^{-4}$.

The session contained a review talk on the "Principles of the RTOF method and Fourier technique" by P.Hiismäki (VTT, Finland), reports on the operating Fourier RTOF diffractometers including "M.SFINKS diffractometer at the Gatchina reactor" by V.Trounov (PNPI, Russia), "The Fourier RTOF neutron diffractometer FSS at the 5 MW research reactor FRG-1" by H.-G.Priesmeyer (Kiel University, Germany), "Performance of the high resolution Fourier diffractometer at the IBR-2 pulsed reactor; latest results" by A.M. Balagurov (FLNP JINR, Russia) and a report on "Calibration of the RTOF mini SFINKS diffractometer for precision structure investigations" by D. Chernyshov (PNPI, Russia).

Table 1 summarizes the parameters of the reported diffractometers in comparison with the conventional TOF diffractometer HRPD at ISIS.

Table 1. Parameters of high resolution TOF diffractometers

Parameter	HRPD RAL UK	m-SFINKS PNPI Russia	FSS GKSS Germany	HRFD JINR Russia
λ	0.9-8	0.9-41.6-4	0.9-12	
Θ	$3 \cdot 10^6$	$1 \cdot 10^7$	$1 \cdot 10^7$	$1 \cdot 10^7$
S	2	4.5	5	2
Ω	0.2	0.09	0.1	0.16
$R \cdot 10^4$	5	20	20	5

λ(Å) is the interval of wavelength, Θ (n/cm^2/s) the neutron flux at the sample position, S(cm^2) the maximal "useful" cross-section of the sample, Ω(sr) the solid angle of the detector assembly, and $R = \Delta d/d$ - the resolution of the diffractometer.

Considering the experience of operating Fourier RTOF diffractometers and the results obtained by their users, we can conclude that today, we have a powerful and effective method for structural investigations with steady state and, especially, with large pulsed sources. This provides an additional argument in favour of the greater importance of higher flux rather than narrower pulse width for effective use of neutron sources.