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TOF diffraction experiments with NEAT at BENSC

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Abstract

We report on a series of experiments performed on the very flexible TOF spectrometer NEAT at the Berlin Neutron Scattering Center, which demonstrates one of the unusual possibilities offered by this instrument: TOF diffraction with incident neutron wavelengths up to at least 20 Å. This is especially suitable for studies of complex systems with large unit cells, as the structural characterization and inelastic scattering measurements can be carried out consecutively, without changing geometry and sample environment.

Keywords: Time-of-flight; Diffraction; Biological structures

NEAT is a high-resolution multichopper time-of-flight spectrometer for inelastic neutron scattering experiments in the region of medium to very small energy and momentum transfers, including elastic and inelastic small angle scattering experiments. Due to the optimized design of the instrument, the data rate of NEAT in standard operation with its single detectors is very comparable to the ILL spectrometer IN5 [1,2]. Another particularity of this spectrometer is to allow for further unique TOF experiments, which have recently been carried out, such as TOF diffraction with long incident wavelengths using the single detectors, elastic and inelastic small-angle scattering with the multidetector at zero angle, or quasielastic critical scattering with high (Q,ω)-resolution on a single crystal with the multidetector at large scattering angle. The last two possibilities concerning the two-dimensional position sensitive multidetector will be reported in a forthcoming more detailed article. In this paper, we focus on the TOF diffraction option which is an easy task for NEAT owing to the great flexibility of its chopper system. Using only the last pair of counter-rotating choppers at low speed, a pulsed white beam is obtained which permits time-of-flight diffraction experiments [3,4]. The chopper speed and the duration of the period have been chosen to permit recording of TOF diffraction patterns with the single detectors, with neutron wavelengths from 1 to 20 Å.

Fig. 1 presents a typical TOF diffraction spectrum, measured with NEAT at $T = 10$ K, of the so-called muscovite "amber" mica which belongs to the layered

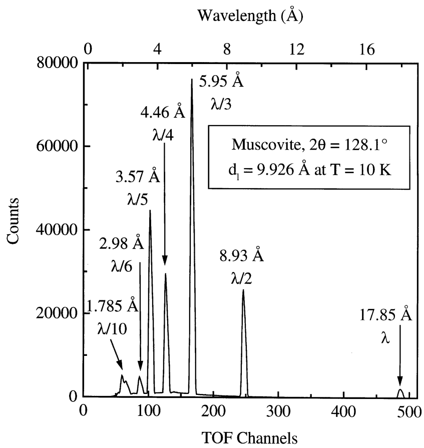

Fig. 1. TOF diffraction pattern of a layered alumino-silicate structure (muscovite, $d_1 = 9.926$ Å) measured with NEAT at $T = 10$ K, showing well-defined reflections up to incident neutron wavelengths of 17.85 Å. These reflections have been used to calibrate precisely the TOF scale in units of wavelength.

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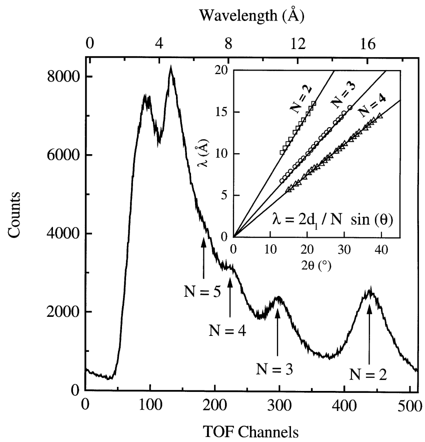

Fig. 2. TOF diffraction pattern of a PM sample equilibrated at 98% RH (D_2O), measured at room temperature with NEAT, showing four orders of lamellar reflections. The inset shows the result of a simultaneous refinement of three orders of lamellar reflections, which leads to an accurate determination of the lamellar spacing constant $d_l = 85.6$ Å.

alumino-silicate structural family. The known value of its d_l-spacing (9.926 Å) [5] has been used to calibrate precisely the TOF scale in units of wavelength for this configuration. As an example to demonstrate the new opportunities given by NEAT and in particular the use of long wavelengths, which are more suitable for studies of samples with large unit cells, we have carried out a series of experiments on purple membrane (PM) multilayer systems. Lamellar reflections up to the fifth order have been measured at low scattering angles at room temperature. Four of them are shown together in Fig. 2 for $2\theta = 22.7°$ for a PM sample equilibrated in the presence of D_2O vapour at 98% RH. This leads to a very precise determination of the lamellar spacing constant d_l, when all the data are analyzed simultaneously as shown in the inset of Fig. 2. Note that the lamellar reflections are seen in a relatively large 2θ-range because of the appreciable mosaic spread (FWHM = 12°) of the oriented PM stacks.

The most important point is obviously, that this crucial structural information can be unambiguously related to the dynamical one, as standard inelastic scattering experiments can follow immediately on the same spectrometer, without removing the sample from the cryostat.

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