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A method of precise profile analysis of diffuse scattering for the KENS pulsed neutrons

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Abstract

An outline of our profile analysis method, which is now of practical use for the asymmetric KENS pulsed thermal neutrons, are presented. The analysis of the diffuse scattering from a single crystal of D₂O is shown as an example. The pulse shape function is based on the Ikeda-Carpenter function adjusted for the KENS neutron pulses. The convoluted intensity is calculated by a Monte-Carlo method and the precision of the calculation is controlled. Fitting parameters in the model cross section can be determined by the built-in nonlinear least square fitting procedure. Because this method is the natural extension of the procedure conventionally used for the triple-axis data, it is easy to apply with generality and versatility. Most importantly, furthermore, this method has capability of precise correction of the time shift of the observed peak position which is inevitably caused in the case of highly asymmetric pulses and broad scattering function. It will be pointed out that the accurate determination of true time-of-flight is important especially in the single crystal inelastic experiments.

1. Introduction

In a conventional profile analysis of coherent elastic and inelastic scattering peaks from single crystal samples, one determines the physical parameters by fitting calculated intensity to the observation assuming a model scattering function. For the data taken by the triple-axis spectrometer, the method of determining, for example, the inverse correlation length from the diffuse scattering from short range order is well established. For the thermal neutrons from the KENS pulsed sources, however, the pulse shape is highly asymmetric and the instrumental resolution function for the single crystal experiments is also considerably asymmetric. Consequently the conventional gaussian approximation does not work for the analysis which needs high accuracy. In order to overcome this, we have proposed a full numerical convolution method [2] by utilizing the Ikeda-Carpenter pulse shape function [3]. This routine was, combined with the least square fitting procedure, used for the resolution correction of the MAX inelastic spectrometer. In this report, we show representative results and point out that this method is indispensable for the calibration of the spectrometer in the case of single crystal experiments. The convolution with the use of the reliable pulse shape function would be the best way of deducing the true time-of-flight (TOF) from the observed peak. We demonstrate the applicability in the case of the diffuse scattering from a deuterium-ordered single crystal of KOD-doped D₂O ice. (For details of the science of this study, one should refer a separate report).

2. Outline of analyses

The procedure is straight forward and similar to the conventional method used in the data analysis on the triple-axis spectrometers. Convolution of the model cross section with the

instrumental resolution characteristics is performed by means of the Monte-Carlo integration (simulation) technique. A nonlinear least square routine (the Levenberg method [3]) is combined for the purpose of fitting the convoluted profile to the observation. As an example, the elastic diffuse peak in D₂O ice is shown, but the procedure for the inelastic scattering is essentially the same. A flowchart of the procedure is shown in Fig. 1.

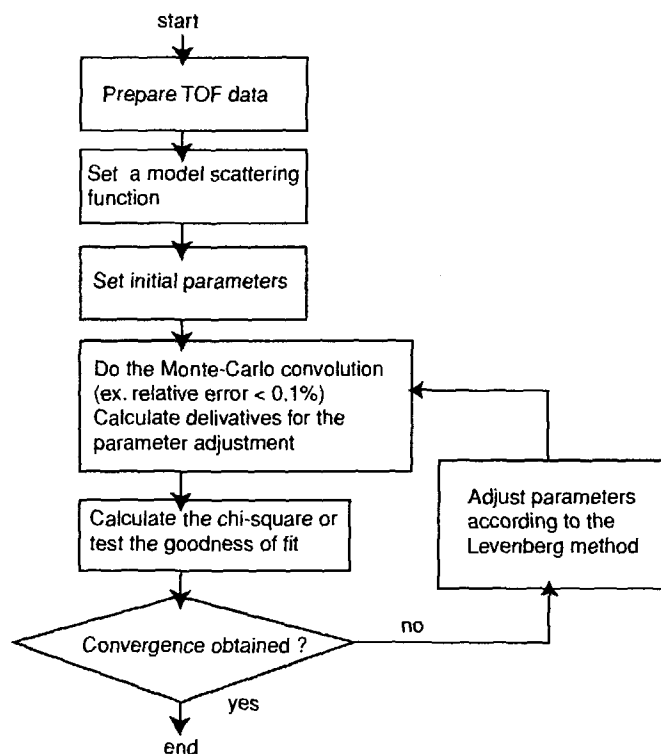


Fig. 1 Flowchart of the analysis.

Prior to the analysis, the profile of the incident neutron pulse is determined by using Bragg peaks of a standard single crystal of Si or PG. Note that the instrumental resolution effect is already included in this observed Bragg peaks. Therefore the deconvolution procedure is necessary in this stage to estimate the adequate profile parameter of the incoming neutrons. Results are shown in Fig. 2. There remains at present, however, some difficulty in reproducing the observed pulses in a wide time-of-flight (TOF) range (see Si (111) case in Fig. 2) with a single set of parameters though the reproduction is sufficient for a limited wave length interval. Next, a model scattering function and initial parameters are set. In the present example as shown in Fig. 3, a Lorentzian form of the scattering function is assumed for the broad profile due to the short range order in the early stage of the ordering process and a squared-Lorentzian plus Lorentzian form was tried for the data taken in the later stage since the single Lorentzian form could not fit the data. With the use of the pulse shape function determined above, the convolution is made by means of the Monte-Carlo multi-dimensional numerical integration (or equivalently the Monte-Carlo ray-tracing method). Combined with the nonlinear least square fitting procedure, the parameters have been determined. The capability of the fitting is satisfactory in spite of the highly asymmetric pulse shape as shown in Fig.3.

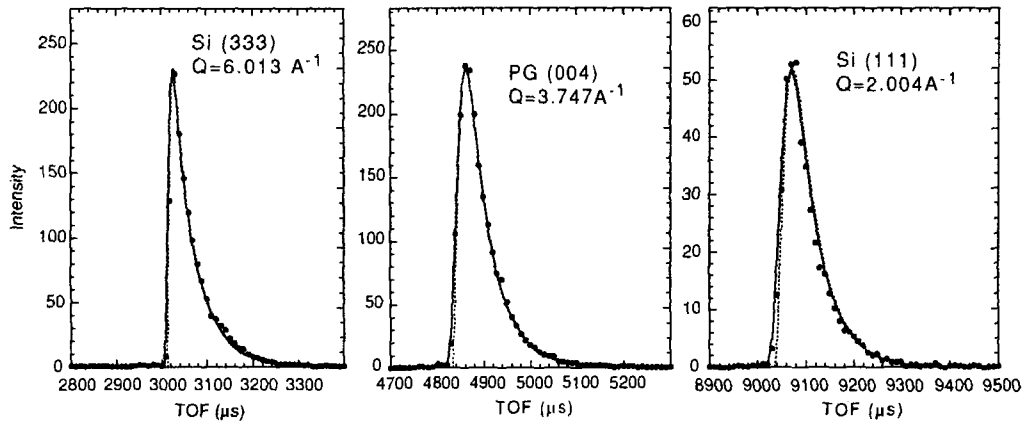


Fig.2 Calibration of the instrumental parameters using sharp Bragg peaks. Dotted lines are the neutron pulses without instrumental broadening effect and the solid line are the convoluted profiles.

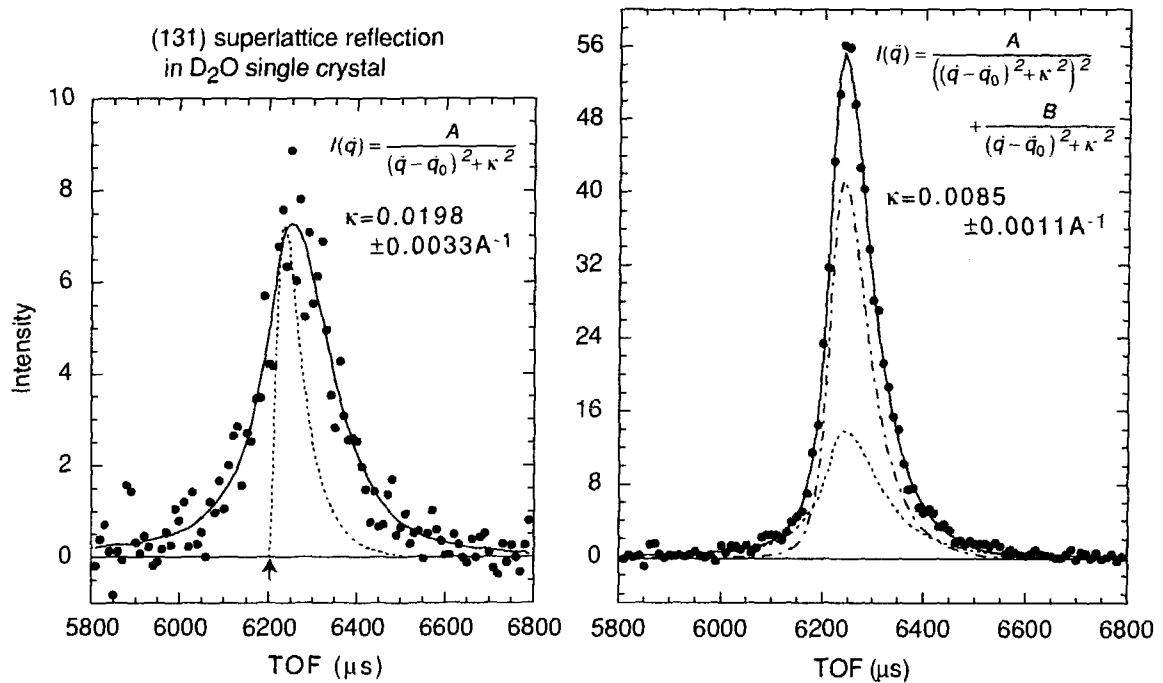


Fig. 3 Result of fitting of the Lorentzian function (left) and the Lorentzian plus squared-Lorentzian function (right). Dotted line in the left figure is the pulse shape of the incoming neutrons and the arrow indicate the true TOF corresponding to $q_0 = 2.921 \text{ \AA}^{-1}$

In the inelastic experiments with single crystal samples on the inverted type inelastic spectrometer like MAX, the energies of the scattered neutrons are usually calibrated by the incoherent elastic peak of Vanadium. Without any correction, the observed peak position does not correspond to true TOF and therefore a proper consideration of the time shift is essential for the accurate scans because the precise setting of the inelastic scans rely on the calibration of the energies of the scattered neutrons. We should emphasize that, since the misalignment of the

spectrometer caused by this kind of time shift results in the systematic errors, the accurate correction is essential for the single crystal experiments.

3. Discussion

We have shown that our method is practical and capable of analyzing the scattering intensities from single crystal samples in the case of the extremely asymmetric pulses as long as an appropriate pulse shape function is provided. The calculation time for the single peak fitting is tolerable even on PCs. Furthermore, this kind of numerical method would be the best way of dealing with the time shift in the observed peak. The method is easy to extend for fitting of two and three dimensional data array. The source codes will be opened after some refinement has been made.

References

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