successfully applied to the determination of the crystal structure of brazilianite [$NaAl_3(PO_4)_2(OH)_4$] (Eggleton & Finney, in preparation).

The author is most grateful to Dr I. M. Threadgold and Dr S. W. Bailey for their helpful criticism and suggestions for improvements to the manuscript. Dr C. W. Burnham & Dr J. W. Tracy kindly permitted the use of their experimental data.

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Resolution of a Triple Axis Spectrometer

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(*Received* 30 *December* 1968)

A new method for obtaining the resolution function for a triple-axis neutron spectrometer is described, involving a combination of direct measurement and analytical calculation. All factors which contribute to the finite resolution of the instrument may be taken into account, and Gaussian or experimentally determined probability distributions may be used. The application to the study of the dispersion relation for excitations in a crystal is outlined.

1. Introduction

An important property of a triple-axis spectrometer is its resolution function, defined as the probability distribution for momentum and energy which a neutron, registered in the counter, has transferred to the sample under investigation. Several papers have treated the resolution of triple-axis spectrometers by various methods; analytically (Collins, 1963; Stedman & Nilsson, 1966; Cooper & Nathans, 1967); graphically (Peckham, Sanderson & Sharp, 1967; Bergsma & van Dijk, 1965) or by direct measurements (Møller, Houmann & Mackintosh, 1968; Møller, 1968). The present paper describes the determination of the resolution by a combination of measurement and calculation, in which no prior knowledge of collimations and mosaic spreads is necessary. Non-Gaussian probability distributions and curvature of the dispersion relation may be taken into account with this method.

Because of finite collimations in the triple-axis spectrometer and the mosaic spreads of the monochromator and analyser crystals, there is, for a fixed position of the spectrometer, a spread of the incoming and scattered neutron wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ around their average values $\mathbf{k}_{10}$ and $\mathbf{k}_{20}$. As a result, there will be a finite probability that the neutron scattering vector $\boldsymbol{\kappa}=\mathbf{k}_1-\mathbf{k}_2$ differs from its average value $\boldsymbol{\kappa}_0=\mathbf{k}_{10}-\mathbf{k}_{20}$, and that the energy transfer $E=E_1-E_2=\hbar^2/2m(k_1^2-k_2^2)$ will differ from the average energy transfer $E_0=\hbar^2/2m(k_{10}^2-k_{20}^2)$. This probability function is called the resolution function $R(\boldsymbol{\kappa}-\boldsymbol{\kappa}_0, E-E_0)$; it is a four-dimensional function. Since the component of $\boldsymbol{\kappa}-\boldsymbol{\kappa}_0$ normal to the scattering plane is not correlated with the other two components of $\boldsymbol{\kappa}-\boldsymbol{\kappa}_0$ or with E, we need only consider the resolution function in the remaining three dimensions, that is, energy transfer, E, and momentum transfer in the scattering plane.

This resolution results from four independent contributions, each of which gives a finite resolution along a line in the three-dimensional $\boldsymbol{\kappa}E$-space. We will denote the vectors along these lines, with length equal to the half-width of the distributions, by $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$, and $\mathbf{X}_4$ [see Fig. 1(*b*)].

$\mathbf{X}_1$ results from the finite collimation of the monochromator system. With zero mosaic spread of the monochromator crystal the probability distribution of the monochromator system is $P_1(\chi_1/X_1)$ along the $\mathbf{X}_1$ direction. Mosaic spread of the monochromator system introduces an independent probability distribution $P_2(\chi_2/X_2)$ along the $\mathbf{X}_2$ direction, so that the total resolution function of the monochromator system is $P_M(\chi_1, \chi_2)=P_1(\chi_1/X_1)P_2(\chi_2/X_2)$. $\mathbf{X}_3$ and $\mathbf{X}_4$ are the corresponding vectors for the analyser system.

2. Calculation of resolution

(1) *Gaussian case*

By the use of the Bragg law $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$ and $\mathbf{X}_4$ are easily calculated (Nielsen & Møller, 1968). Below are given the projections of $\mathbf{X}_t$ on the E axis, X_{tE}, and on the $\boldsymbol{\kappa}$ plane, $X_{i\boldsymbol{\kappa}}$, and the orientation of $X_{i\boldsymbol{\kappa}}$ in the $\boldsymbol{\kappa}$ plane.

$$X_{1E}=2E_{10}\cot\theta_M\,\frac{\sigma_1\sigma_2}{\sqrt{\sigma_1^2+\sigma_2^2}}\,,$$

$$X_{1\kappa}=-\frac{k_{10}}{\sin\theta_M}\,\frac{\sigma_1\sigma_2}{\sqrt{\sigma_1^2+\sigma_2^2}}\,, \qquad (1)$$

$$u_1=\theta_M\,;$$

$$X_{2E}=2E_{10}\cot\theta_M\,\frac{\sigma_2^2-\sigma_1^2}{\sigma_2^2+\sigma_1^2}\left[\frac{4}{\sigma_1^2+\sigma_2^2}+\frac{1}{\eta_m^2}\right]^{-1/2},$$

$$X_{2\kappa}=\frac{k_{10}}{\sin u_2}\,\frac{2\sigma_2^2}{\sigma_1^2+\sigma_2^2}\left[\frac{4}{\sigma_1^2+\sigma_2^2}+\frac{1}{\eta_m^2}\right]^{-1/2}, \qquad (2)$$

$$\tan u_2=\tan\theta_M\,\frac{2\sigma_2^2}{\sigma_2^2-\sigma_1^2}\;(0<u_2\leq\pi)\,;$$

$$X_{3E}=2E_{20}\cot\theta_A\,\frac{\sigma_3\sigma_4}{\sqrt{\sigma_3^2+\sigma_4^2}}\,,$$

$$X_{3\kappa}=\frac{k_{20}}{\sin\theta_A}\,\frac{\sigma_3\sigma_4}{\sqrt{\sigma_3^2+\sigma_4^2}}\,, \qquad (3)$$

$$u_3=\theta_A\,;$$

$$X_{4E}=2E_{20}\cot\theta_A\,\frac{\sigma_3^2-\sigma_4^2}{\sigma_3^2+\sigma_4^2}\left[\frac{4}{\sigma_3^2+\sigma_4^2}+\frac{1}{\eta_A^2}\right]^{-1/2},$$

$$X_{4\kappa}=\frac{k_{20}}{\sin u_4}\,\frac{2\sigma_3^2}{\sigma_3^2+\sigma_4^2}\left[\frac{4}{\sigma_3^2+\sigma_4^2}+\frac{1}{\eta_A^2}\right]^{-1/2}, \qquad (4)$$

$$\tan u_4=\tan\theta_A\,\frac{2\sigma_3^2}{\sigma_3^2-\sigma_4^2}\;(0<u_4\leq\pi)\,.$$

The notation is given in Fig. 1(*a*). σ_i denotes the half-width of the angular neutron distribution transmitted through a collimator and η_i denotes the half-width of the mosaic distribution. θ_M and θ_A are the Bragg angles of monochromator and analyser respectively.

We now wish to find the instrumental width of a neutron group in a scan along the vector **c** through a dispersion surface $E(\mathbf{q})$ (see Fig. 2).

Because the four linear distributions $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$ and $\mathbf{X}_4$ are independent, we can (in the Gaussian approximation) find the instrumental width (in units of **c**), by treating each of these four distributions separately and calculating the square root of the sum of their squared contributions. The resulting instrumental width is therefore

$$W=\left(\sum_i W_i^2\right)^{1/2}=\left[\sum_i\left(\frac{\mathbf{n}\,.\,\mathbf{X}_i}{\mathbf{n}\,.\,\mathbf{c}}\right)^2\right]^{1/2}; \qquad (5)$$

n is the normal to the dispersion surface.

If we know all probability distributions $\mathbf{X}_i$, we can calculate the instrumental resolution for any scan from (5). If all collimations σ_1, σ_2, σ_3, σ_4 and the mosaic spreads η_M and η_A are known, the vectors $\mathbf{X}_i$ may be calculated by the use of formulae (1) to (4).

If required, the resolution ellipsoid (half value contour surface of $R(\boldsymbol{\kappa}-\boldsymbol{\kappa}_0, E-E_0)$ can be determined by calculating its projection on any direction **c**, by the use of equation (5) with $\mathbf{c}=\mathbf{n}$.

(2) *Non-Gaussian case*

If the probability distributions along $\mathbf{X}_i$ are found experimentally to be non-Gaussian (see § 3), we can find the instrumental resolution for any scan in the following way: we now interpret $\mathbf{X}_i$ as a characteristic length of the probability distribution $P_i(\chi_i/X_i)$ along $\mathbf{X}_i$. Each of these distributions is treated separately, giving a contribution to the resulting scattered intensity of the same form as $P_i(\chi_i/X_i)$. If the variable along the scanning direction **c** is denoted v and W_i is defined from (5), the individual contributions to the scattered intensity are $P_i(v/W_i)$. The resolution is now found from the following formula

$$P(v)=\iiint P_1\left(\frac{v_1}{W_1}\right)P_2\left(\frac{v_2}{W_2}\right)P_3\left(\frac{v_3}{W_3}\right)\times P_4\left(\frac{v-v_1-v_2-v_3}{W_4}\right)dv_1dv_2dv_3$$

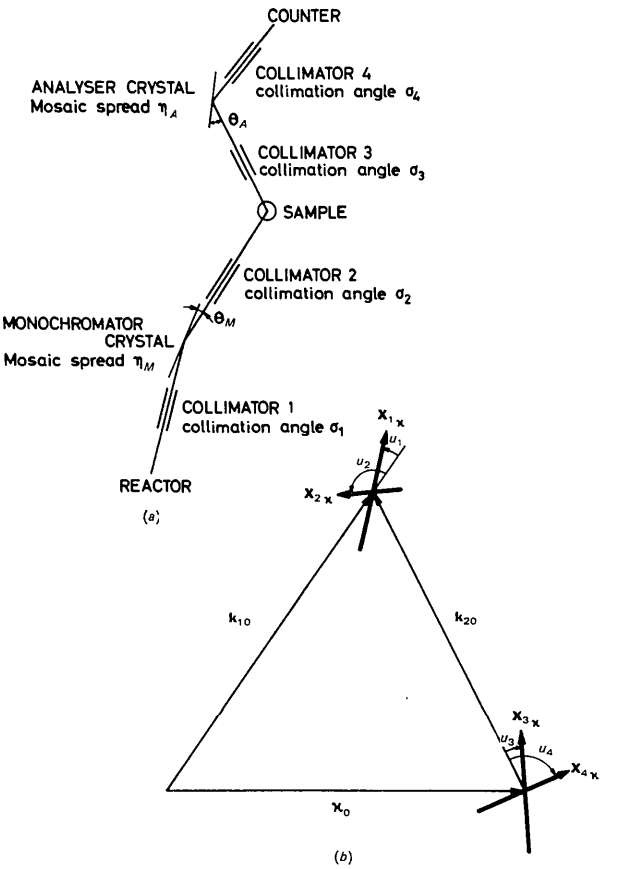

Fig. 1. (*a*) Schematic diagram of the triple-axis spectrometer, (*b*) vector diagram showing the projections on the κ plane of the four independent contributions to the resolution resulting from finite collimation in the monochromator system, $\mathbf{X}_1$, mosaic spread in the monochromator, $\mathbf{X}_2$, finite collimation in the analyser system, $\mathbf{X}_3$ and mosaic spread in the analyser crystal $\mathbf{X}_4$.

or

$$P(v)=\int P_M\left(\frac{v_M}{W_M}\right) P_A\left(\frac{v-v_M}{W_A}\right) dv_M\,, \qquad (7)$$

where

$$P_M\int\left(\frac{v_M}{W_M}\right)=\int P_1\left(\frac{v_1}{W_1}\right) P_2\left(\frac{v_M-v_1}{W_2}\right) dv_1$$

and

$$P_A\left(\frac{v_A}{W_A}\right)=\int P_3\left(\frac{v_3}{W_3}\right) P_4\left(\frac{v_A-v_3}{W_4}\right) dv_3 \qquad (8)$$

are the contributions to the resolution from monochromator and analyser, respectively.*

(3) *Mosaic spread of the sample*

Mosaic spread of the sample may be taken into account by introducing a probability distribution which lies in a plane perpendicular to the scattering vector $\boldsymbol{\kappa}_0$. If this probability distribution can be written as a product of distributions in the scattering plane, $P_{5h}(\chi_{5h}/X_{5h})$, and perpendicular to the scattering plane, $P_{5v}(\chi_{5v}/X_{5v})$, we may define two characteristic lengths X_{5h} and X_{5v} of these two distributions and use formula (5) to calculate the contribution to the neutron group. We must now use four-dimensional **n** and **c** vectors.

However, the sample may not be a single crystal, but it may consist of a few crystals with small differences in orientation. In this case the vertical and horizontal distributions P_{5h} and P_{5v} are correlated and we must measure the total distribution $P_5(\chi_{5h},\chi_{5v})$ by the method described in § 3. This distribution is then projected onto the normal, **n**, to the dispersion function. This gives the contribution $P_s(v)$ to the scattered intensity measured in a scan perpendicular to the dispersion function. For a scan in a general direction, **c**, $P_s(v)$ must be divided by the projection of **c** on **n**. The total resolution $P'(v)$ is now given by

$$P'(v)=\int P(v')P_s(v-v')dv'\,. \qquad (9)$$

(4) *Non-planar dispersion surface*

We have so far assumed a planar dispersion surface over the extension of the resolution. Let us now consider a constant $\mathbf{q}_0$ scan with wave vector $\mathbf{q}_0$ along a symmetry direction and take into account the curvature of the dispersion surface. We write the dispersion surface around $\mathbf{q}=\mathbf{q}_0$

$$E(\mathbf{q})=E_0+\alpha_1(q_1-q_{10})+\beta_1(q_1-q_{10})^2 +\beta_2q_2^2+\beta_3q_3^2, \qquad (10)$$

where q_1, q_2 and q_3 are the components of **q** along three symmetry directions. The scattered intensity from the planar dispersion relation $E(\mathbf{q})=E_0+\alpha_1\,(q_1-q_{10})$ is found from equation (5) to be

$$P_t\left(\frac{E_0-E}{X_{tE}-\alpha_1X_{tq_1}}\right). \qquad (11)$$

With the dispersion relation (10) the scattered intensity is obtained from (11) by changing the energy coordinate from E to E' where

$$E_0-E'=E_0-E-(\beta_1X_{tq1}^2+\beta_2X_{tq2}^2+\beta_3X_{tq3}^2) \times\left[\frac{E_0-E}{X_{tE}-\alpha_1X_{tq_1}}\right]^2$$

where X_{tq_1}, X_{tq_2}, X_{tq_3} and X_{tE} are the components of $\mathbf{X}_t$ along $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$ and **E**.

* It is assumed that the transmission probabilities for the collimators are still Gaussian. If this is not correct, we may, instead of using formulae (8), measure the probability distributions for the monochromator and the analyser directly. A simple calculation using the Bragg law gives their variation with spectrometer setting.

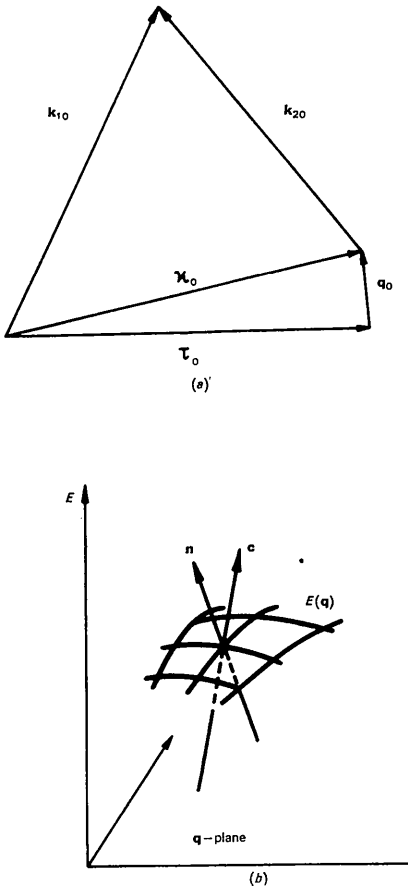

Fig. 2. (*a*) Vector diagram for the excitation of a phonon (or magnon) of wave vector $\mathbf{q}_0$ (*b*) Dispersion surface $E(\mathbf{q})$ in the three-dimensional $\mathbf{q}E$ space. **n** is a vector normal to the dispersion surface and **c** is an arbitrary scanning direction.

3. Measurement of resolution

As we shall now show, it is possible to measure directly:

(i) the resolution function $R(\boldsymbol{\kappa}-\boldsymbol{\kappa}_0, E-E_0)$ for the spectrometer set at $E_0=0$ and $\boldsymbol{\kappa}_0=\boldsymbol{\tau}_0$, a reciprocal lattice vector of the sample;

(ii) the individual probability distributions $P_t(\chi_t/X_t)$.

This allows a very accurate determination of the resolution function for the triple-axis spectrometer.

The observed intensity $I(\mathbf{q}_0, E_0)$ as a function of the settings of the spectrometer $\mathbf{q}_0$ and E_0 is obtained by folding the cross section for the scattering process, $\sigma(\mathbf{q}, E)$, and the experimental resolution function, $R(\mathbf{q}-\mathbf{q}_0, E-E_0)$,

$$I(\mathbf{q}_0, E_0) = \int\int R(\mathbf{q}-\mathbf{q}_0, E-E_0)\sigma(\mathbf{q}, E)d\mathbf{q}dE\,. \quad (12)$$

In particular, if measurements are performed on a Bragg reflexion, for which $\sigma(\mathbf{q}, E) \simeq \delta(\mathbf{q})\delta(E)$ we find the intensity

$$I^B(\mathbf{q}_0, E_0) \simeq R(-\mathbf{q}_0, -E_0)\,. \quad (13)$$

The resolution function $R(\mathbf{q}, E)$ can therefore be measured by mapping the Bragg reflected intensity as a function of the settings of the spectrometer.

We can make the resolution width of the analyser system small in comparison with the resolution of the monochromator system by the use of first-order reflexion in the monochromator crystal and third- or higher-order reflexion in the analyser crystal.

By measuring the Bragg reflected intensities as a function of the settings of the spectrometer, we now measure the resolution resulting from the probability distributions $P_1(\chi_1/X_1)$, $P_2(\chi_2/X_2)$, $P_{5h}(\chi_{5h}/X_{5h})$ and $P_{5v}(\chi_{5v}/X_{5v})$. Since the direction of $\mathbf{X}_1$, $\mathbf{X}_{5h}$ and $\mathbf{X}_{5v}$ are known, we can determine $P_1(\chi_1/X_1)$, $P_{5h}(\chi_{5h}/X_{5h})$ and $P_{5v}(\chi_{5v}/X_{5v})$ by measuring the intensity in scans along these directions. If the horizontal and vertical probability distributions P_{5h} and P_{5v} are correlated, their resulting distribution can be determined by measuring the Bragg reflected intensities in a plane perpendicular to τ_0. The remaining distribution $P_2(\chi_2/X_2)$ and the unknown direction of $\mathbf{X}_2$ may be determined by measuring the peak intensity in scans parallel to $\mathbf{X}_1$ in the plane defined by $\mathbf{X}_1$ and $\mathbf{X}_2$. This plane intersects the $\boldsymbol{\kappa}$ plane in a line perpendicular to $\mathbf{k}_{10}$ and the slope of the plane is

$$\alpha = 2E_{10}/k_{10}\,. \quad (14)$$

If necessary, correction for the influence of the analyser resolution can be made. The resolution with which, for instance $P_1(\chi_1/X_1)$, is measured is [from equation (5)]

$$\left[\left(\frac{\mathbf{n}\,.\,\mathbf{X}_3}{\mathbf{n}\,.\,\mathbf{X}_1}\right)^2 + \left(\frac{\mathbf{n}\,.\,\mathbf{X}_4}{\mathbf{n}\,.\,\mathbf{X}_1}\right)^2\right]^{1/2}, \quad (15)$$

in units of $\mathbf{X}_1$. In equation (15) $\mathbf{X}_3$ and $\mathbf{X}_4$ are, of course, the small values found when the analyser is in a higher-order reflection, and

$$\mathbf{n} = \begin{vmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \mathbf{E} \\ X_{2q1} & X_{2q2} & X_{2q3} & X_{2E} \\ X_{5hq1} & X_{5hq2} & X_{5hq3} & X_{5hE} \\ X_{5vq1} & X_{5vq2} & X_{5vq3} & X_{5vE} \end{vmatrix};$$

$\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$ and $\mathbf{E}$ are vectors along the axis in the four-dimensional coordinate system.

$P_3(\chi_3/X_3)$, $P_4(\chi_4/X_4)$ and the direction of $\mathbf{X}_4$ can be determined in a similar way, by making the resolution of the monochromator system small in comparison with the resolution of the analyser system.

Summary

We have shown how a combination of calculation and experimental measurements may be used to determine the resolution function of a triple-axis spectrometer for arbitrary energy and momentum transfers.

As an example, the resolution width of the neutron distribution resulting from phonon or magnon scattering from a given sample may be obtained in the following manner. The individual contributions, $P_i(\chi_i/X_i)$, to the spectrometer resolution function including effects of mosaic spread of the sample, are measured for one spectrometer setting by the method described in § 3. Since the variation of $P_i(\chi_i/X_i)$ with spectrometer setting is known from § 2, we may calculate $P_i(\chi_i/X_i)$ for any spectrometer setting, and we can use equations (5) or (6) to calculate the resolution width of any scan through a dispersion surface. The individual probability distributions are determined experimentally and do not therefore have to be Gaussian. The calculated resolution function for zero energy transfer may be checked experimentally from equation (13).

The authors are grateful to J. Als-Nielsen and A. R. Mackintosh for many valuable discussions.

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